Lappeenranta University of Technology
Faculty of Technology
Department of Mathematics and Physics

A GENERALIZED 1D PARTICLE TRANSPORT METHOD FOR CONVECTION DIFFUSION REACTION MODEL

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Supervisors: Prof. Ph.D. Heikki Haario and Prof. Ph.D Matti Alatalo.
Examiners: Prof. Ph.D. Heikki Haario and Prof. Ph.D Matti Alatalo.

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Makungu James
Punkkerikatu 3D 1
53850 Lappeenranta
Makungu.M.James[at]lut.fi

Abstract

Lappeenranta University of Technology
Department of mathematics and Physics
Makungu James

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This work is devoted to the development of numerical method to deal with convection diffusion dominated problem with reaction term, non - stiff chemical reaction and stiff chemical reaction. The technique is based on the unifying Eulerian - Lagrangian schemes (particle transport method) under the framework of operator splitting method. In the computational domain, the particle set is assigned to solve the convection reaction subproblem along the characteristic curves created by convective velocity. At each time step, convection, diffusion and reaction terms are solved separately by assuming that, each phenomenon occurs separately in a sequential fashion. Moreover, adaptivities and projection techniques are used to add particles in the regions of high gradients (steep fronts) and discontinuities and transfer a solution from particle set onto grid point respectively.

The numerical results show that, the particle transport method has improved the solutions of CDR problems. Nevertheless, the method is time consumer when compared with other classical technique e.g., method of lines. Apart from this advantage, the particle transport method can be used to simulate problems that involve moving steep/smooth fronts such as separation of two or more elements in the system.

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ABBREVIATIONS

MOL	Method of Lines
PDE	Partial differential equations
PTM	Particle transport method
MM	Meshless method
TVD	Total variation diminishing
FE	Finite element
FDM	Finite difference method
CFL	Courant-Friedrichs-Levy condition
CDR	Convection diffusion reaction
1D	One dimensional
2D	Two dimensional
3D	Three dimensional
ODE	Ordinary differential equation
FTCS	Forward time central spatial
CFD	Computational fluid dynamics
ENO	Essential non-oscillatory
SPH	Smoothed particle hydro-dynamics
m	m^{th} time step
Γ	Boundary condition of computational domain
$[a, b]$	Computational domain
$f(\phi)$	Monotonic increasing function
i	i^{th} grid point in the computational grid
u	Convective velocity in the computational domain
$C(x, t)$	Unknown concentration or function
$Sgrid$	Stationary grid points in the domain
N	Number of particles
C	Vector of the moving components of a mixture
D	Diffusion coefficient
G_i	Signal value on the i^{th} interval of grid
M	Number of time steps

Contents

CHAPTER ONE

INTRODUCTION

1.1 General Introduction

The numerical simulation technique of convection-diffusion-reaction models has been a subject of the active research during the last thirty years [5]. The development of the new techniques and methods able to solve the models still now days attracts substantial attention. Especially, this concerns problems on flow or transfer of materials. Therefore, in this study material transfer processes are classified into three categories: forced convection (or advection) due to the movement of material (concentration) from one region to another region, for instance in heat system, convection is the transfer of heat by the actual movement of the warmed matter. This implies that, advective term depends on flow velocity [36]. The second process is called diffusion (or dispersion) which is caused by the movement of material (system) from the region of high concentration to the region of low concentration or heterogenic distribution of concentration in material and lastly is a reactive term, that describes possible processes like adsorption, decay and reaction of the substances with other components or it's a process that results in the inter-conversion of chemical substances (Ghani, 2007). These processes are combined together and form a single model, which explains a physical system that can undergo convection, diffusion and reaction process within a system. Quantitatively, convection-diffusion-reaction model is a mathematical model that describes how the concentration of the substance distributed in the medium changes under the influence of these three processes. Although these processes occur at different time scales, the resultant numeric scheme should account for this interaction in order to achieve the required numerical criteria of stability, convergence and consistency (Hoffman). These phenomena can be found in the following physical system, one, crystal growth, that occurs from the addition of new atoms, ions or polymers strings into the characteristics arrangement of a Crystalline Bravais Lattice. Second, biological engineering for the application of engineering principles and technologies to the medical field, it combines the design and problem solving skills of engineering with medical and biological sciences to improve healthcare diagnosis and treatment. Third, food processing as the set of methods and techniques used to transform raw ingredients into food or to transform food into other forms for consumption by humans or animals either in home or by the food processing industry and many others which use this model. However, solving this model by hand becomes difficult due to the iterations carried out during the computational process (simulation). Fortunately the advanced technology of digital computing makes possible for the model to be solved or computed easily, because some of the softwares were designed to meet with these difficulties. Apart from that, using this tool (computer) we can investigate and predict the behavior of the model at any time step in the area of computational domain. Hence, the appropriate numerical methods have initiated a specialized current in the field of computational fluid dynamics which approximates the solution of the model.

It has been reported that when diffusion dominates in a system of physical processes (strong movement of flux from high concentration to low concentration), the standard finite difference method (FDM) or the finite element method (FEM) produces satisfactorily results [21]. On the other hand, when convection governs the process, numerical instabilities like oscillations (non-physical features) or numerical dispersion appear on the solution approximated by these two schemes (Al-Lawatia *et al.*, 1999). These difficulties in the computational domain are caused by the nature of the system itself. In reality, for the system dominated by convection, features such as discontinuities, or high values of the gradients caused by initial condition, inflow condition and reaction rate should be observed in the solution. Therefore, classical numerical techniques normally produce unwanted features in the approximated solutions. To avoid these difficulties one can separate convection, diffusion and reaction terms under the framework of operator splitting approach and resolve each of them with a most appropriate solver. The output from each step becomes the initial state for the next step and it is achieved or done by dividing the time interval into small time steps. This method has the desirable advantage of alleviating the restrictions on the Courant number, thus allowing for large time steps [38]. On the other hand this method has difficulty in conservating mass and treating general boundary conditions.

Recent studies have shown that the spatial adaptivity has improved the resolution of the solution discontinuities, by refinement of a computational mesh in the regions of singularities (discontinuous or high values of the gradients) indicated by the gradient or the residual magnitude of the solution [14], or in the regions of the maximum error estimated after each time step [32]. From this point of view, adaptivity is similar to the re-meshing procedure needed in the Lagrangian methods (adding nodes/grids in the present nodes). As longer as adaptivity procedure is very powerful tool, it leads to mesh reconstruction, in both dimensional and increase the time for computation if one use hand. The convection diffusion reaction models in this study represents a system that allows its material (concentration) to move along one direction e. g. flow of fluid with pollutants in a tube, river etc and dominate the outward movements. Hence, 1D will be strongly considered in this research and not 2D and 3D because of the nature of the system represented by the model. In simple cases, analytical techniques have been used to solve the models of the physical systems modeled by partial differential equations, e.g., diffusion model, convection model, coupled convection-diffusion model and many others. Unfortunately, many of the partial differential equations that represent the system do not have exact solutions (closed forms). On the other hand, numerical techniques have been used as an alternative approach on the challenged problems to resolve the solutions in discrete form.

For CDR model dominated by diffusion and insignificant convection has a solution when approximated by finite difference or finite element (Eulerian schemes). The same model when dominated by convection and insignificant diffusion has a solution if semi-Lagrangian method is applied. Unfortunately the model does not have a clear approximated solution when both processes (convection and diffusion) are dominated or significant. Therefore this study intends to bridge this gap by developing a technique that will bring a solution when both convection and diffusion are dominated. Especially, we study cases with multicomponent stiff chemical reaction systems (the systems of different components with different reaction rates). Such problems are significant in chemical industries, especially in chromatographic separation processes. In a system, some components have different reaction rate (some react faster than others), then, the tracking (information) of every component in the system at different time step require a fast algorithm to analyze them. This is due to the fact that, some of them might be used up before the computational time has reached.

The overall objective of this study is to unify particle transport method (Eulerian-Lagrangian) for convection and diffusion dominated with a reaction model in 1D. Furthermore, the thesis is organized as follows;
Chapter two represents the literature review that includes analytical methods and numerical methods. In chapter three, the particle transport method is described together with methodology. Chapter four contains the numerical results and the evaluation of the methods. The conclusions are summarized in section five.

CHAPTER TWO

LITERATURE REVIEW

2.1 Introduction

Different studies have been conducted in the computational fluid dynamics (convection diffusion and reaction system) along one, two or three dimensional domain. In this chapter, we present briefly some methods or schemes that have been used by various researchers for the approximation of solutions of the models numerically. We will concentrate on the computation of convection diffusion reaction model (reaction-transport) by numerical approach and not much in the analytical techniques.

There have been both analytical and numerical approximation of solution for investigating the solution of partial differential equations in the field of computational fluid dynamics (CFD) [10]. The treatment of the model is often difficult analytically; this is due to the fact that some of the partial differential equations (models) do not typically have known exact solutions. Many scholars have come up with different approaches for computing various models in fluid dynamics field. These include Finite difference schemes (e.g., Lax-Wendroff methods, Upwind method, Mac cormack method, Crank-Nicolson method), Finite volume methods (e.g., Godunov's schemes, High-resolution scheme, MUSCL method, Riemann solver), Finite element methods (e.g., h-p-Fem, Meshfree methods, Petrov-Galerkin FEM methods, Streamline diffusion FEM methods. The Eulerian-Lagrangian localized adjoint methods ELLAM), Method of lines and level set method [14]. On the other hand, some of these schemes produce better results when they are applied to some models, but others have the tendency of generating some spurious oscillations or numerical diffusion to the solution at a particular time step [31]. The comparison of these schemes associated with numerical solutions will be analyzed in this section.

2.1.1 Analytical Methods.

2.1.2 One-Dimensional Linear Convection Equation.

Physical systems in which convection is a predominant phenomenon are commonplace in science and engineering [22]. On the other hand, this is one of the most significant physical phenomena in the mechanics of fluids and in the heat and mass transfer processes. It also has a primary importance in many problems of biomechanics and plasma physics. The question that arises during the computational process is the development of artificial oscillations, numerical diffusion or high values of the gradient to the approximated solution [6]. In general these systems are relatively difficult to analyze because they exhibit steep moving fronts and even discontinuities that must be resolved with good accuracy method if the important characteristics of these systems are observed and understood. For simplicity, the model of pure linear advection is analysed analytically by assuming that the system is ideal, which means the viscosity term is neglected in the system. On the other hand, the system without viscosity develops sharp fronts and discontinuities in the mathematical solution. In the real world, thermal fluids systems in general are dispelled, meaning that the viscosity, however small it is, is present and plays an important role in smoothing out the sharp fronts [13]. Nevertheless, a pure convection problem offers a system for analysis, and for understanding of the nature of convection models [28]. In this section we describe some techniques applied for solving a physical system problem analytically. The following is the pure linear convection partial differential equation herein, describes the movement of a physical quantity such as pollutants which associated with the flow of fluid in respective to time and spatial. The model takes the following form

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} = 0 \tag{1}$$

where u is the convection velocity and is taken to be positive constant along the computational domain for the sake of simplicity, but it can be negative constant as well as the function of x and t [20]. Also $C(x,t)$ is the unknown function of (x,t), it represents the value of the physical quantity (concentration) at x and t respectively. Using the method of characteristics, we consider a particular curve $x = x(t) \in [a,b]$ at time $t \in [0,T]$. Then, the total derivative of $C(x,t)$ with respect to time is governed by the chain rule

$$\frac{dC(x,t)}{dt} = \frac{\partial C(x,t)}{\partial t} + u\frac{\partial C(x,t)}{\partial x} = 0 \tag{2}$$

The equation (1) is written in the Eulerian form and we assume that the velocity field $\frac{dx}{dt} = u(x,t)$ is known. The interpretation of (1) is that the scalar function C is constant along trajectories. Each of these trajectories is entirely determined by $u : [a,b] \to R$. The semi-Lagrangian method integrates the Lagrangian form (2) of the convection along trajectories as given below;

$$\int_{C(x_0,\ t_0)}^{C(x,\ t_0+\Delta t)} dC(x,t) = 0 \tag{3}$$

where by Δt is the time step size ($\Delta t > 0$) and x_0 is the upstream point. The point x_0 provides the unique location of the particle at time t_0, which by traversing along its trajectory arrives at x at time $t_0 + \Delta t$. Therefore at particular time, $C(x, t_0 + \Delta t) = C(x_0, t_0)$. For a finite set $P = x_1, x_2, \cdots, x_n \in [a,b]$ of current particles or nodes, the semi-Lagrangian method requires at each time step $t \to t_0 + \Delta t$ computing a vector $C_P^{t_0+\Delta t} = C(x_1, t_0 + \Delta t), \cdots, C(x_n, t_0 + \Delta t)$ of new concentration values at time $t_0 + \Delta t$ from the corresponding vector $C_P^{t_0}$ of the previous time step. Given that at $t_0 = 0$ the values in $C_P^{t_0}$ are given by the initial condition. In [20] the computational of each new concetration value $C(x, t_0 + \Delta t)$ $x \in P$, is given as follows.

(i) Compute the characteristic curves $\widehat{x} = u(x,t).t + x_{0i}$, $i = 1, 2, \cdots, n$

(ii) Interpolate $C(\widehat{x}, t)$

(iii) Advect by letting $C(x, t_0 + \Delta t) = C(\widehat{x}, t)$. As the method of the characteristic explained here, the solution (physical quantity) at any period of time remain constant (mass conservation), what is changing is only position of the quantity. Apart from that, method of characteristic solves some coupled physical problems such as convection-reaction regardless the computational domain is not complex. On the other hand, the structure of the domain determine whether or not the technique can be applied to the model. Furthermore, this is basic technique of all the time which has been applied in fluid dynamic problems. But analytical solutions to the transport equations (fluid dynamic problems) are rarely possible for the following reasons;

(i) complexity of the convective velocity

(ii) many models are represented in three dimensional

(iii) many models are strongly coupled and non-linear partial differential equations
(iv) in practical engineering problems, the solution domain are almost always complex [8].

These problems cause the method of characteristic to be selective for some models in the field of fluid dynamics. Nevertheless, some of models can be made amenable (accepted) to analytical solutions when simplified through assumptions. Limitation of this idea is that, the solution computated by employing these assumptions to the model lead to the unclear solution.

2.1.3 Numerical methods

2.1.4 Lax - Wendroff Method

In this section we describe some of the predominant techniques applied in computational fluid dynamic problems and their weakness. Typically we consider techniques used in approximation of solutions of the models representing physical phenomena. As one of the oldest technique, Lax- Wendroff approach is a scheme for solving approximately systems of hyperbolic conservation laws [8]. It has played a historic role in computational problems and simply it is a second-order accurate in both space and time. The method has two steps; the first step, calculates values of $c(x,t)$ at half time step $t_{n+\frac{1}{2}}$ and half grid points $x_{i+\frac{1}{2}}$. In the second step values at t_{n+1} are calculated using the data for t_n and $t_{n+\frac{1}{2}}$. Therefore, in one space dimensional, the scheme for convection equation read as;

$$C_i^{n+1} = C_i^n - \frac{\Delta t}{\Delta x}.\left(C_{i+\frac{1}{2}}^{n+\frac{1}{2}} - C_{i-\frac{1}{2}}^{n+\frac{1}{2}}\right) \tag{4}$$

where C_i^{n+1} is a vector of the physical quantity at a next time step. One of the earliest extensions of the scheme is the Richtmyer two-step Lax-Wendroff method, which is the form [18], with the numerical flux given as;

$$C_i^{n+1} = \frac{1}{2}\left(C_i^n + \hat{U}_i^+\right) + \frac{1}{2}\left(\frac{dt}{dx}\left(\hat{f}_{i-1}^+ - \hat{f}_i^+\right)\right). \tag{5}$$

Although the second-order Lax-Wendroff scheme produces reasonable approximation to the smooth profile, the method is unstable on the sharp front due to the formation of non-physical oscillation in the numerical solution [4]. On the other hand, oscillations in the numerical solution near steep gradients in the profile reduced when Richtmyer scheme implemented to the problem with moving steep fronts.

2.1.5 Upwind schemes

The upwind schemes represent a class of numerical discretization methods for solving hyperbolic partial differential equations [1]. The upwind schemes attempt to discretize hyperbolic partial differential equations by using differencing biased in the direction determined by the sign of the characteristic speeds. The first order-upwind scheme is given by;

$$C_i^{n+1} = C_i^n - \alpha \left(C_{i+1}^n - C_{i-1}^n \right) \tag{6}$$

where by $\alpha = u\frac{\Delta t}{\Delta x}$. Many works have been done using this scheme and one of the examples is the work of Godunov-type central-upwind scheme [6]. Although the schemes approximate the solution of the physical systems when the Courant-Friendrichs-Levy condition is less than one ($\alpha = u\frac{\Delta t}{\Delta x}$), features such as numerical diffusions in the solution are always observed. On the other hand, if the initial condition has large gradient, the first-order upwind scheme introduces severe numerical diffusion in the solution. These errors are also observed if one use second-order upwind scheme or third-order upwind scheme. Nevertheless, third - order has less diffusive compared to the second order accurate scheme, but suffer from the spurious oscillations in the vicinity of the solution.

2.1.6 Upwind (FDM) and Lax-Friedrichs scheme

2.1.7 Explicit Scheme for one Dimensional transport equation

The one-dimensional transport equation for zero reaction has written as;

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} = D\frac{\partial^2 C}{\partial x^2} \tag{7}$$

$x \in (a,b)\,, t \in (0,T)$. Where C is a passive scalar which is being convected with a known velocity $u\,(x,t)$ in the computational domain and being diffused. To examine the behavior of computational solutions of equation (7) is assumed that u and D

are constants. The transport equation is strictly parabolic and requires the initial and boundary conditions. However, when $\frac{u}{D}$ becomes large the first two terms in (7) would be expected to dominate. Then the transport equation will demonstrate behavior similar to the convection equation. It may be recalled that exact solutions of the convection equation are typically wave motions that propagate with no damping (reduction in amplitude). According to this scheme, the problem has been solved using the forward time central spatial ($FTCS$). Therefore, the FTCS scheme applied to (7) produces the algebraic equation as shown below;

$$\frac{C_j^{n+1} - C_j^n}{\Delta t} + u\frac{C_{j+1}^n - C_{j-1}^n}{2\Delta x} - D\frac{C_{j-1}^n - 2C_j^n + C_{j+1}^n}{\Delta x^2} = 0 \tag{8}$$

which as an algorithm, can be written $C_j^{n+1} = (s + 0.5p)\, C_{j-1}^n + (1 - 2s)\, C_j^n + (s - 0.5p)\, C_{j-1}^n$ where $s = D\frac{\Delta t}{\Delta x^2}$ and $p = u\frac{\Delta t}{2\Delta x}$. In this algorithm, the solution in each time step is simulated using the previous data. Unfortunately, there are limitations on the size of Δt and Δx. If they are chosen wrongly, the method ($FTCS$) becomes unstable, it simply blows up. For this reason, some literatures have been used a difficult form called an implicit method. This is unconditionally stable with all Δt and Δx. However, if Δt and Δx are chosen poorly or large, it may give a bad answer, but it will not explode. Using this technique, the equation (7) can be written as

$$\frac{C_j^{n+1} - C_j^n}{\Delta t} + u\frac{C_{j+1}^{n+1} - C_{j-1}^{n+1}}{2\Delta x} - D\frac{C_{j-1}^{n+1} - 2C_j^n + C_{j+1}^{n+1}}{\Delta x^2} = 0 \tag{9}$$

$$C_j^{n+1} - C_j^n + p\left(C_{j+1}^{n+1} - C_{j-1}^{n+1}\right) - s\left(C_{j-1}^{n+1} - 2C_j^{n+1} + C_{j-1}^{n+1}\right) = 0 \tag{10}$$

$$(-p - s)\, C_{j-1}^{n+1} + (1 + 2s)\, C_j^{n+1} + (p - s)\, C_{j+1}^{n+1} = C_j^n \tag{11}$$

From equation (10), we see what looks like three unknowns $(C_{j-1}^{n+1}, C_j^{n+1}, C_{j+1}^{n+1})$ at the time step $(n + 1)$. For $j = 0$ to J, where the boundary conditions are $C(a, t)$ and $C(b, t)$ for all time $t > t_0$ defined. If the boundary conditions together with the initial conditions are known, then the equation (10) can be expressed as a matrix equation in linear algebra as shown below;

$$Q = \begin{pmatrix} (1+2s) & (-p-s) & 0 & 0 & 0 & \cdots & 0 \\ (-p-s) & (1+2s) & 0 & 0 & 0 & \cdots & 0 \\ 0 & (-p-s) & (1+2p) & 0 & 0 & \vdots & 0 \\ 0 & 0 & (-p-s) & 0 & 0 & \cdots & 0 \\ \vdots & 0 & 0 & 0 & 0 & \ddots & 0 \\ 0 & 0 & 0 & 0 & (-p-s) & (1+2s) & (-p-s) \\ 0 & 0 & 0 & 0 & 0 & (1+2s) & (-p-s) \end{pmatrix},$$

$$W = \begin{pmatrix} C_1^{n+1} \\ C_2^{n+1} \\ C_3^{n+1} \\ \vdots \\ C_{J-1}^{n+1} \\ C_{J-2}^{n+1} \\ C_{J-1}^{n+1} \end{pmatrix}, M = \begin{pmatrix} C_1^{n} + (p+s)C_0^{n+1} \\ C_2^{n} \\ C_3^{n} \\ \vdots \\ C_{J-1}^{n} \\ C_{J-2}^{n} \\ C_{J-1}^{n} + (p+s)C_J^{n+1} \end{pmatrix},$$

$$M = Q * W \tag{12}$$

In even more compact matrix, equation (10) can be expressed as equation (12), where the capital letters indicate the entire matrix. It shows that we have the inverse of the $(J-1)*(J-1)$ matrix Q, we can solve for the all C_j^{n+1} with the simple multiplication;

$$\begin{cases} QC_j^{n+1} = C_n^n \\ Q^{-1}QC_j^{n+1} = Q^{-1}C_j^n \\ C_j^{n+1} = Q^{-1} \end{cases} \tag{13}$$

The matrix Q is called tridiagonal because it has only three diagonals of $(-p-s)$, $(1+2s)$ and $(-p-s)$. It is called diagonally dominant because $(1+2s) > |-p-s| + |-p-s|$, the absolute value of each element of the diagonal is greater than the sum of the absolute values of the elements on the same row off the diagonal. This second property assures that the solution to equation (11) will exist [6]. It is known that the solution to the space-centered explicit scheme does not oscillate only when peclet number ($pe = u\frac{\Delta x}{D}$) is less or equal to 2 and the CFL condition $p \leq 1$ (Richard,*et al 2000*). Furthermore, for the linear hyperbolic PDE, $\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} = 0$, $x \in (a,b)$,

$t \in [0,T]$ this can be viewed as a limiting case of $D \to 0$ in equation (7), the corresponding scheme to the linear convective problem is $\frac{C_j^{n+1}-C_j^n}{\Delta t} + u\frac{C_{j+1}^n - C_{j-1}^n}{2\Delta x} = 0$ so this is unconditional. The upwind FDM uses a one-sided finite difference in the upstream direction to approximate the advection term in the transport PDE (7) and can be expressed as follows (assuming $u > 0$);

$$\frac{C_i^{n+1} - C_i^n}{\Delta t} + u\frac{C_{i+1}^n - C_{i-1}^n}{2\Delta x} - D\frac{C_{n+1}^n - 2C_i^n + C_{i-1}^n}{\Delta x^2} = 0 \tag{14}$$

The Lax-Friedrichs scheme is given by

$$\frac{C_i^{n+1} - \frac{C_{i+1}^n + C_{i-1}^n}{2}}{\Delta t} + u\frac{C_{i+1}^n - C_{i-1}^n}{2\Delta x} - D\frac{C_{n+1}^n - 2C_i^n + C_{i-1}^n}{\Delta x^2} = 0 \tag{15}$$

and it obtained by replacing C_i^n in the first term in equation (8) by its mean value, for the purpose of stabilize a numerical scheme from the spurious oscillations in the vicinity of the solution singularities. Therefore the two schemes, the Upwind (FDM) and Lax-Friedrichs minimize the non-physical oscillations present in scheme applied to the algorithm (8) and generate stable solutions even for every complicated multiphase and multicomponent flows. It can be shown that the Upwind FDM scheme is actually a second-order approximation to equation (7) with a modified diffusion $D(1 + \frac{pe}{2}(1-p))$, while the Lax-Friedrichs scheme is a second-order approximation to equation (7) with an extra numerical diffusion $\frac{\Delta x^2}{2\Delta t}(1-p^2)$ (Ewing, 1984). Although these techniques (Upwind FDM, Lax-Friedrichs) approximate the solution of the transport equation (convection diffusion), some errors still exist if one use these techniques. For instance, using Lax Friedrichs scheme strong numerical diffusion (dispersion) to the approximated solution and non physical oscillations observed at the vicinity of the approximated solution respectively. In general the two schemes are conditional due to the fact that if $s = D\frac{\Delta t}{\Delta x^2} > 0.5$, both of them would not converge to the solution.

In [40] non - physical oscillations can be precluded by using two techniques. The first method is done by adding the so called shock - capturing viscosity or stabilizing term which acts as diffusion aimed to smooth possible oscillations in the regions of singularities. Second technique is done by smoothing the solution after each step of the simulation according to the value of artificial viscosity which generally depends on the second derivative of the solution. The solution can be smoothed either globally over the whole computational domain or, to avoid overdiffusing in the regions of the smooth solution, only in the vicinity of singularities, which can be located by the gradient of the solution. Moreover, special care should be taken to avoid a downgrade of the accuracy in the smooth part of the solution, which may be caused by an excessive numerical diffusion.

2.1.8 Method of lines (MOL)

In general many works concerning computational of fluid dynamics have been done through the use of method of lines. This is a computational approach for solving PDE problems of the form of equation (7) that proceeds in two separate steps; first, spatial derivatives e.g., C_x, C_{xx} are approximated using, for instance, the following $O(\Delta x^2)$ finite difference operators (FD) or finite element (FE) techniques while time is kept continuous. Second, the resulting system of semi-discrete ODEs in the initial variable is integrated in the time t. In [42], the method of line applied in the approximation of solution of CDR model is described as follows. Initially, the first and second spatial derivatives $\frac{\partial C}{\partial x}$ and $\frac{\partial^2 C}{\partial x^2}$ respectively are replaced by second-order, centered FD at grid point i.

$$\frac{\partial C_i}{\partial x} = -u\frac{C_{i+1} - C_{i-1}}{2\Delta x} + O\left(\Delta x^2\right) \qquad i = 1, 2, \cdots, N \tag{16}$$

$$\frac{\partial^2 C_i}{\partial x^2} = \frac{C_{i+1} - 2C_i + C_{i-1}}{\Delta x^2} + O\left(\Delta x^2\right) \tag{17}$$

$$f(x, t, C) = f(x_i, t, C_i) \tag{18}$$

where by N represent grid points separated uniformly by a distance dx in the computational domain. Second, by substituting these equations $(16) - (18)$ in the CDR model with $u = a$ give a system of N ODEs;

$$\frac{dC_i}{dt} = -a\frac{C_{i+1} - C_{i-1}}{2\Delta x} + D\frac{C_{i+1} - 2C_i + C_{i-1}}{\Delta x^2} + f(x_i, t, C_i) \quad i = 1, 2, \cdots, N. \tag{19}$$

Note, spatial grid index i has the values corresponding to a system of N initial value ODEs that can be integrated by any ODE integrator. However, equation (19) needs auxiliary condition, in order to be solved; these are initial condition (IC) required for t and two boundary conditions (BCs) are required for x. These might be, for example;

$$C(x_i, 0) = f(x_i) \tag{20}$$

$$C(0, t) = f(t) \tag{21}$$

$$\frac{\partial C(x,t)}{\partial x} = 0 \tag{22}$$

Nevertheless, the author in [25] [12] has used C_0 and C_{N+1} to be the fictitious points (outside the spatial domain) that must be included in the ODEs for $i = 1$ and $i = N$ and are calculated by using central spatial FD grid. In the method of lines, the spatial differencing must be done by the user while the time discretization and error control is handled by the ODE software. Overall, the effort to develop a new simulation is reduced, since a good deal of existing high-level software can be used. Although, method of lines reduces the partial differential equations into more simple ordinary differential equations by discretizing all but one of the independent variables, the method still have problems. For instance, the method of lines cannot be used directly on purely elliptic equation, such as Laplace's equation, because the approach uses time integrator and Laplace's equation is not time dependant. Apart from this limitation, the method requires too much storage for each of the unknown quantities being computed. For example, the GEAR ODE code in its standard form requires that a minimum of [13] storage locations (plus any possibly required matrix storage) be available per ODE being solved [33]. This would be quite excessive to the person interested in solving a $3-D$ time dependant problem who is used to needing only several locations per point in the problem. What one needs to keep in mind is the fact that in its standard form, GEAR may use up to a 12^{th} order time integration formula which would require [33] locations just to store the past history data. Clearly for many PDEs use of this type of formula would be absurd. Another drawback of the approach is that, the software used for integration is too inefficient. Hence, an appropriate software or more efficient program should be constructed in order to eliminate these kinds of limitations. In fact, we have seen several cases where the general purpose software has actually solved a PDE problem in less than $1/1000-th$ of the time required by a novice user generated code specifically designed for the particular problem at hand. In another way, the method of lines still powerful method in approximation of solutions of PDE problems. Furthermore, spurious oscillations and numerical instabilities [19] can result when equation (19) is employed and the velocity u is large or the grid spacing is not sufficiently small, but can be eliminated by using nonsymmetric $O(\Delta x)$ operators for convection term or by introducing numerical terms in the discretized equation [11].

2.1.9 Meshless Methods

Several computational works of fluid dynamics have been done using meshless or mesh free technique. It is different approach compared with mesh-based approach. In a meshless method a set of scattered nodes are used instead of meshing of domain. In [37] a numerical technique (mesh free) shows that the schemes is significantly more time consuming compared with mesh-based due to complex shape function with a high order of continuity which demand specially constructed kernel for their evaluations. Furthermore, meshless technique uses variations radial functions (i.e. the Gaussian functions, the cubic or quadratic spline functions) as a powerful tool for scattering data interpolation problem. On the other hand, the use of moving particles may facilitate the application of Lagrangian methods to the transport problems since there is no need in the re-meshing procedure to maintain a sufficient quality of mesh. For these reasons meshless schemes are very suitable for the problems with moving solutions and discontinuities [4], free-boundary problems and problems in complex geometries. Among numerous mesh free methods, the following methods have widely gained popularity in computational fluid dynamics; the Smooth Particle Hydrodynamics method, formulated initially for astrophysical and quantum mechanics applications, the Vortex- in - cell method based on the Lagrangian vorticity-velocity formulation of the governing equations and a smoothing kernel function. One of the recent works in the computational of convection-diffusion model has used Smoothed particle Hydrodynamics approach (the word 'particle' does not mean a physical mass; instead, it refers to a region in space). This is meshfree method that is based on the Lagrangian approach. In this method, each computational point carries field variables such as velocity, pressure, temperature and moves with the fluid in time. Smoothed Particle Hydrodynamics (SPH) was first presented by Lucy [1]. In the work the author used a kernel interpolation to evaluate the first-order derivative. For second-order derivatives, three different schemes are frequently used; double summation scheme, second-order kernel derivation scheme and difference scheme.

CHAPTER THREE

METHODOLOGY

3.1 Convection Diffusion with Reaction.

In this chapter we look at the ways to attain the stated objectives. To develop an accurate PTM in $1D$ for convection diffusion dominated model and to validate the PTM developed when applied in stiff chemical reaction consisting of several components (three components A, B and F are considered here). We start with convection diffusion reaction model, as stated above a model is derived from continuity equation that links the combination of convection with diffusion and reaction term (*Kohno et al*, 2000). However, the model has an ability to switch between parabolic and hyperbolic types with respect to the domination of diffusion or convection terms. This behavior of the model brings unexpected result in the approximation of the solution of the model using numerical techniques (e. g. Eularian method) due to the presence of either artificial oscillations or excessive numerical diffusion in the solution. The problems observed to the approximated solution due to this shift from one behavior to another behavior can be eliminated by applying mixed Eulerian-Lagrangian techniques (particle transport method).

In this work, the unified Eulerian-Lagrangian approach (particle transport method) will be developed for the approximation of the solution of convection diffusion dominated model on each time step within the framework of operator splitting approach. While operating on the basis of the Lagrangian concept, this kind of schemes keeps the advantage of the presentation of the solution on a fixed Eulerian grid. The Eulerian-Lagrangian methods essentially rely on the idea of exact transport plus projection. The first step may be accomplished with either forward or backward tracking of the characteristics while the second step can be done by projection of solution from particle system into grid. The methods mentioned above (forward or backward and projection) will be done by creating some algorithms and implement them by using MATLAB 7.3.0 ($R2007a$) on 2x3GHz Dual Core Xenon $8Gb$ desktop PC.

3.2 Mathematical model and operator splitting technique

The first part in this work we define a convection diffusion model with reaction term by considering that the reaction term should also be significant in the process. In the second part, we define a model with three components reacting (nonstiff chemical reaction and stiff chemical reaction) while they are advecting and diffusing in the domain. Therefore, the Lagrangian-Eularian method (PTM) will be explained step by step in both cases (part one and part two), i.e, the way it solves or approximates the solution of the system (model). On the other hand, the two terms of the model (convection and diffusion) will be considered to be significant to each other to the model. Hence, the convection diffusion reaction model is defined as

$$\frac{\partial C}{\partial t} + (u\nabla) \times C = D\Delta C + f(x,t,C) \qquad in \ \ (a,b) * (0,T) \tag{23}$$

$$C\,(x,0) = C_0\,(0) \qquad in \ \ (a,b) \tag{24}$$

$$\alpha_{in} C\,(a,t) + \beta_{in} \frac{\partial C}{\partial x}\,(a,t) = C_{in}\,(a,t) \qquad on \ \ \Gamma_{in} * (0,T) \tag{25}$$

$$\alpha_{out} C\,(a,t) + \beta_{out} \frac{\partial C}{\partial x}\,(a,t) = C_{in}\,(a,t) \qquad on \ \ \Gamma_{out} * (0,T) \tag{26}$$

where $C = C\,(x,t)$ is unknown function or a function that describes the physical quantity such as mass or concentration, x belongs to the bounded domain (a,b) and t belongs to the time interval $(0,T)$. The convective velocity field $u = u(x,t)$ is given in $(a,b) \times (0,T)$ and is solenoidal (constant) which is $\nabla \times u = 0$ in (a,b) at any moment of time. In this study the convective velocity will be taken as a positive and non-dependant of spatial and time along the computational domain, this will simplify the construction of characteristic curves in the $x - t$ plane. For an equation (23) to be solved, initial condition (24) at $t = 0$ and boundary conditions $(25) - (26)$ should be provided. Γ_{in} and Γ_{out} are the inflow and outflow parts of the domain boundary. The solution of this initial boundary value model $(23) - (26)$ keeps its value along the characteristic curves which are defined by the ordinary differential equation;

$$\frac{dx}{dt} = u(x,t). \tag{27}$$

The equation (27) forms basic concepts of semi-Lagrangian algorithms. The computational process of the model is initiated through the following steps, the first step is done by creating the stationary mesh in the domain (a, b) or grid, and the grid can be either uniform or non-uniform, so in this work only uniform grid will be considered. The second step is achieved through the transport of the exact solution from the grid and carried out by moving the system of the particles (coordinate or numerical points). The system of particles are defined by using grid nodes and the particles are not necessary to be placed at all nodes. Therefore, only small amount of particles are needed at the beginning and the initial adaptivity algorithm adds particles in the regions where the initial condition has high gradients or steep front using the linear interpolation (gradient technique). The process of adding particles in the vicinity of the solution is done, so that the numerical computational can capture the resolution of the approximated solution in these regions.

3.3 The meshless technique (particle transport method)

The meshless technique will use system of particles instead of grid in the computational domain, that will reduce the computational cost of the physical problems modeled by partial differential equations . It has two concepts; the first one is called discontinuities and/or high gradients of the solution function convected by an incompressible flow determined by the initial and inflow boundary conditions. Therefore the improvement should be done at the initial step and near the inflow part of the boundary only. The second idea will be done by controlling the density of the particles by means of an adaptivity procedure. Hence, in this section we describe a number of ways to ensure that the model is solved with this new technique (PTM). The following steps herein are required for the computational of the model and are given as follows;
(i) adaptive distribution of the particles

- initial distribution of particles

- movement of the particle set and the inflow adaptivity

(ii) solving of the convection - reaction subproblem using the splitting approach technique in the time interval on the particle set created in part (i).

- adaptivity by solution

(iii) projection of the solution from the particle system onto the grid. Recall that, the solution of the model is represented on the grid.
(iv) solving of the diffusion subproblem on the grid using method of lines. This step will use the solution of stage (iii) as an initial condition.

3.3.1 Distribution of particles using adaptivity procedure

3.3.2 Initial distribution of particles

The positions of the particles are created by using the set of grid nodes. Furthermore, using adaptivity procedure as an algorithm, the particles will be added in some regions of the domain, especially in the vicinities of steep fronts and discontinuities. These two areas of the solution will be shown by using gradient of the initial condition. Apart from this, the areas where the initial condition is smooth require some attention if we want to get a good and reasonable accuracy approximation solution. The smooth areas are indicated by the second derivatives of the solution. In this work, adaptivity procedure has two initial algorithms used in addition of particles, for the vicinities and discontinuities an algorithm called steep front adaptivity is used and for smooth areas of the solution an algorithm called smooth adaptivity is applied. Hence, linear interpolation is used to approximate the gradient as well as the second derivatives of the solution on each particle. Initially, the exact solution should be known i.e. initial function (initial condition) $C(x,0) = C_0(0)$, then, from this function we can interpolate it on each grid node (the value of the initial condition on each particle) and gradients (signal values). Then, the distribution of particles is done by creating an algorithm using these signal values and is given as follows. Let G_i be the signal value of the initial solution function on the i^{th} interval and G_{mean} and G_{max} , respectively, the mean and maximum of the considered signal value on the whole length of the domain. Then, add N_{add} new points to the system of particles on interval using the rule;

$$N_{add} = \begin{cases} 0 & \text{if } G_i <= G_{mean} \\ N_{max} & \text{if } G_i = G_{max} \\ f_1(G_i) & \text{otherwise} \end{cases} \tag{28}$$

where G_i is the gradient (signal value) in i^{th} interval. N_{max} is the maximum number of particles added to a particular interval, normally between 5 and 10, f_1 is a continuous function increasing from 0 up to N_{max}. The value of G_i in each interval of the particle system is calculated by taking the absolute of the ratio between two adjacent values of the initial function and their distance between them. Since the gradient of a linear interpolation is a constant vector on each interval of the grid, the absolute value of it yields a unique value of the sharp indicator on the considered interval.

The particle position is created by using stationary grid on the domain; these particles do not have to be placed at all nodes but, for example at each m^{th} node. Therefore, the initial algorithm for creation of particles has explained below.

(i) Generate the random distribution of stationary grids on the domain L.

- Stationary Grid = linspace (0, L, n), where n is the number of grid points, 0 and L are the lower and upper boundary of the computational domain respectively.

(ii) Create the indices from 1 to the length of stationary grid and substract one or add one by jumping m steps, m = 2 or 3

- Index = 1: m: length (Stationary Grid) - 1;

- Index = [index (:); length (stationary Grid)];

(iii) Generate the particles (numerical points) with respective to their indices

- Particle set = Stationary Grid (index).

(iv) Evaluate or interpolate the values of the initial condition in all the indices that represent the positions of the particle set

- Value in each particle = feval (initial function, particle set, parameters).

Where by $feval$ calculates the values of the function on the particle set and the argument parameters represent the position of initial function.
(v) Compute the gradient in every interval (spatial interval) and solve for the mean of the gradients and the maximum gradient

- Gradient = $\frac{C_{i+1}-C_i}{x_{i+1}-x_i}$;
- Mean of the gradient = $\sum \left|\frac{G_i}{nn}\right|$

nn is the total number of the gradients in the domain.
(vi) Adaptive to the portions/regions with high gradients can be done as follows;
If G_i is less than or equal to G_{mean} then $N_{add} = 0$
If G_i is equal to G_{max} then $N_{add} = N_{max}$
If G_i is in between G_{mean} and G_{max} then,
$N_{add} = fix(N_{max} * \frac{G_i - G_{mean}}{G_{max} - G_{mean}}) + 1$.
N_{add} is the number of particles added in one interval of the domain and the term fix used to approximate the number of particles in the whole number.

- New particles = adaptivity (old particles, old values of the function, N_{max}, h_{min});

h_{min} indicates the minimum distance between two added particles.
(vii) Compute the values of the function on the new added particles

- New values = feval (initial function, new particles, parameter).

(viii) Display the values of the function calculated (old and new particles)

- Particles = [old particles (:); new particle (:)]

(ix) Put the indices by sorting the particles along the domain (old and new particles)
(x) Display the values of the function on the indices.

- Final values on the particles = values (indices);

The procedures listed above helped to balance between high resolution of singularities (steep front and discontinuities) and small computational costs of the initial condition function. On the other hand, the above steps densitify the particle set in the areas of special interest of the initial condition function.

3.3.3 Movement of the particle set and the inflow adaptivity

Initially, all the particles are assigned the values of the initial condition function $C(x, 0)$ at the respective locations. The initial condition function $C(x, 0)$ provides the data to the given model and it is an exact solution at $t = 0$. During the movement process, all the particles carry these values along the lines called characteristic curves and deposit them to new positions at time $t > 0$. Then, the new positions of the particles at time interval $[t_{n-1}, t_n]$, $n = 1, 2, \cdots, N$ obtained by integrating equation (27) and it becomes the function of (x, t_n). This function provides the new position of any particle at any time interval, if it is integrated properly using either Runge-Kutta technique or any ODE solver technique. Here, Runge-Kutta has used to integrate the equation (27). The inflow adaptivity procedure takes care on the inflow boundary part of the domain. At the time where the particle system moves (simulation time) the inflow boundary part of the domain lose particles due to the convective transport.

In this case, inflow adaptivity adds new particles on this portion and at the same time the values of the inflow function are computed on these new particles. The node or particle x_0 on the inflow boundary receives the values of the boundary function (inflow function) at every time step.

The interval between x_0 and the closest node x_1 adapted similarly to the initialization step as shown above. By using the know function values at the point x_0 and x_1 we linearly interpolate on the interval $[x_0, x_1]$ and compute the signal value

(absolute gradient). If the gradient value becomes greater than $\frac{1}{h}$, where h is the distance between x_0 and x_1, then a new point $x_{\frac{1}{h}}$ is assigned the value of the boundary function with the corresponding time shift. Then, this procedure is repeated for intervals $[x_0, x_{\frac{1}{h}}]$ and $[x_{\frac{1}{h}}, x_0]$ and so on, until the length of the intervals become very small or the signal value becomes less than $\frac{1}{h}$. The same applies to the smooth inflow function; the smooth adaptivity is applied under the condition of directional derivative using three points $p_0, p_{\frac{1}{2}}, p_1$ as starting points to obtain a quadratic interpolation. Therefore, using Matlab routine the inflow adaptive algorithm for addition of particles on the inflow portion of the boundary can be done as follows;
(i) Introduce a new particle x_0 on the inflow part of the domain after the time shift.
(ii) Compute the value of the inflow function $C_{in}(x_0, t)$ on the new particle.
(iii) Add particles between the new particle x_0 on the inflow portion and the closest particle x_1 (initial adaptivity).
(iv) Compute the values of the inflow function $C_{in}(x, t)$ on the added particles between x_0 and x_1 (projection technique).
The particles beyond L of the computational domain are not considered in simulation at any time step. Therefore, this algorithm is always repeated for every time step in the computational domain and improves the resolution of the inflow function. If more than one inflow functions are coming to the inflow portion, then the new particle introduced on the inflow portion assigned the information or values/data of all inflow functions. Finally, the initial condition function $C(x, 0)$ together with the inflow function values are now assigned on the particle system (transport of the exact solution), and this process is followed by integrating the reaction subproblem on the particle system as explained in the next section.

3.3.4 Solving of the reaction subproblem

The integration of reaction subproblem achieved by converting equation (23) using operator splitting technique into the total time derivative and take the form given below;

$$\frac{dC}{dt} = \frac{\partial C}{\partial t} + (u \times \nabla) = f\left(x, t, C\right) \tag{29}$$

$$\frac{dC}{dt} = f\left(x, t, C\right) = k \times C \tag{30}$$

where k is the rate of reaction of C. Then, the solution obtained after integrating the equation (30) (ODE) by using stiff solver method along characteristics curve given by equation (27), provides the final solution of the convection reaction subproblem. Here, the reaction solution becomes an addition source of solution singularities. For more than one components reacting in the computational domain, equation (30) modified as;

$$\begin{aligned} \frac{dC_1}{dt} &= k_1 \times C_1 \times \cdots \times C_n \\ &\vdots \\ \frac{dC_n}{dt} &= k_n \times C_1 \times \cdots \times C_n \end{aligned} \tag{31}$$

On the other hand, the solution of convection reaction subproblem acts as the initial condition of the diffusion subproblem. The parabolic operator of diffusion, in contrast to convection, it implies smoothing of the solution and generally improves the solution for applied numerical technique. In this work, the effect of large diffusion coefficient and large convective velocity to the system will be examined or tested.

3.3.5 Adaptivity by solution

As mentioned in part (3.3.4), the reaction solution is an addition source of solution singularities. Hence, another algorithm called adaptivity by solution needed for an addition of particles in order to improve the solution obtained by integrating equation (30) and it done as follows;

(i) Add particles N_{max} with distance of h_{min} apart according to the rule given below;

$$N_{add} = \begin{cases} 0 & \text{if } G_i <= G_{mean} \\ N_{max} & \text{if } G_i = G_{max} \\ f_1(G_i) & \text{otherwise} \end{cases} \tag{32}$$

(ii) Compute the values of the function on the new particles (projection method);

(iii) Arrange the old particles and the new particles in the computational domain by ascending order (this carried out by indices);

(iv) Assigned the solution of reaction subproblem on these particles;

Furthermore, the computation of the final solution on the grid is carried out by another algorithm after projecting the solution (solution of reaction subproblem) from the particle system onto the grid basing on the linear interpolation as explained in the next section.

3.3.6 Projection of the solution from the particle system onto the grid

For converting solution of convection reaction subproblem from particle system onto grid form, the projection procedure which is based on linear interpolation is applied. It connects between grid and the particles or between the particle set and the new points introduced by adaptivity. This process yields second-order spatial accuracy for smooth solutions in the maximum norm [40]. In the regions of the shocks only first-order accuracy can be achieved. However, adaptivity in the PTM approach reduces this error by using a dense set of the particles in such regions. Therefore, the projection procedure (algorithm) is summarized as follows;

(i) Identify the position of particle system in the computational domain using indices $e.g., j = 1$ to the length of the particle system.

(ii) Assign the solution on the particle system obtained after the reaction part C_j

(iii) Identify the position of grid in the computational domain using indices $e.g., i = 1$ to the length of the grid (number of grid).

(iv) If the grid point x_i in the computational domain coincide with particle point x_j, then assign the solution of particle point x_j to the grid point x_i.

(v) If the absolute distance between x_i and x_j is less than or equal to 1×10^{-10}, then assign the solution of particle point x_j to the grid point x_i.

(vi) If the absolute distance between x_i and x_j is greater than 1×10^{-10}, then apply the linear interpolation to compute the solution C_i to the x_i and is given as;

- $$C_i = C_{j-1} + (x_i - x_{j-1}) \times (\frac{C_{j-1} - C_j}{x_{j-1} - x_j})$$

Hence, these steps applied to transform a solution of reaction subproblem onto grid system and ready for the last computation of the model.

3.3.7 Solving of the diffusion subproblem on the grid using method of lines

The solution of reaction subproblem which has transformed onto the grid system acts as the initial condition of the diffusion subproblem stated below;

$$\frac{\partial C}{\partial t} - D \times \Delta C = 0 \tag{33}$$

Since, equation (23) has first derivative in temporal and second derivative in spatial, then one initial condition and two boundary conditions should be provided for further computation of the model. As stated from part 3.3.4, the initial condition for diffusion subproblem obtained from reaction subproblem. For the boundary conditions, three kinds fit the equation (23) namely Dirichlet condition, Neumann condition and Robin condition. This implies that Dirichlet boundary condition specifies the values a solution needs to take on the boundary of the domain, Neumann boundary condition specifies the values that the derivatives of a solution is to take on the boundary of the domain while Robin boundary condition specifies a linear combination of the values of a function and the values of its derivative on the boundary of the domain [16]. In this part an initial condition together with two boundary conditions are considered i.e., Dirichlet and Neumann boundaries respectively in association with method of line. For simplicity, the method of lines has used to approximate the second derivative in spatial by applying the finite difference method, while the first derivative in temporal remain unchanged.

In order to fulfill the requirement of method of lines, the computational domain should be discretized into grid for assigning the values of the initial condition as well as the boundary conditions. In general, discretization process in computational domain can be done into two categories; the first technique is called uniform discretization , i.e., the separation distance between two adjacent grid points should be maintained at the constant number throughout the computational domain, second approach is called non-uniform discretization , this implies that the distance apart between two adjacent grid points is not necessary to be equal in the computational domain. In this work only uniform spatial has used for discretization of domain.

Furthermore, the system of ordinary differential equations obtained after the finite difference process are integrated by using either Euler method or Runge-Kutta solver. The main concept of diffusion operator in the model is to smooth some unwanted/spurious oscillations around the vicinities of the solution that arise in the approximation of solution of the convection reaction subproblem. On the other hand, diffusion operator improves the final solution of the CDR model. Therefore, spatial second derivative of diffusion subproblem has two steps to be approximated on the discretization grid points (this is based on the 4^{th} - order space discretization).

Hence, the 4^{th} - order space discretization (step one and two) will be used to approximate the spatial second derivative in finite form for the diffusion term in every grid point along the computational domain. In the next chapter, the convection diffusion reaction models with one component, three components (nonstiff) and three components (stiff) will be analyzed using the methodology explained in chapter three.

CHAPTER FOUR

NUMERICAL ANALYSIS OF THE MODELS

4.1 Convection Diffusion model

A convection diffusion dominated equation is used as a first test for the particle transport method. Solution at each time step is compared with the solution by the method of lines. The second part described the applications of the particle transport method for the computation of nonstiff chemical reactions and stiff chemical reactions or kinetics with three components in the computational domain. Furthermore, the solutions of the nonstiff chemical reactions are compared with the solutions of method of lines too. The following system is considered;

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} = D\frac{\partial^2 C}{\partial x^2} + f(x,t,C) \tag{34}$$

$$C(x,0) = \begin{cases} 2 & \text{if } 0.3 \leq x \leq 0.6 \\ 0 & \text{otherwise} \end{cases} \tag{35}$$

$$C(0,t) = 1 \tag{36}$$

$$\frac{\partial C}{\partial x}(L,t) = 0 \tag{37}$$

$$f(x,t,C) = -kC \tag{38}$$

where $u = 0.1msec^{-1}$, $L = 1m$, $k = 0.5sec^{-1}$, $\Delta t = 0.02$, $D = 0.01m^2sec^{-1}$ and 50 number of grid points in the computational domain.

The simulation with the particle transport method is done according to the algorithm presented in the preceding section (chapter three). Since the convective velocity is constant then, it has the following simple analytical solution;

$$\frac{dx}{dt} = u(x,t) = u \tag{39}$$

Hence, by integrating equation (39) throughout the computational domain, it provides the solutions that describe the trajectory lines along the $x - t$ plane as shown in the Figure 1

$$\int_{x_0}^{x(t)} dx = \int u dt \tag{40}$$

$$x(t) = ut + x_{0i} \tag{41}$$

$i = 1, 2, 3, \cdots, n$

where by n is the number of grid points, equally spaced distributed in the domain of computational.

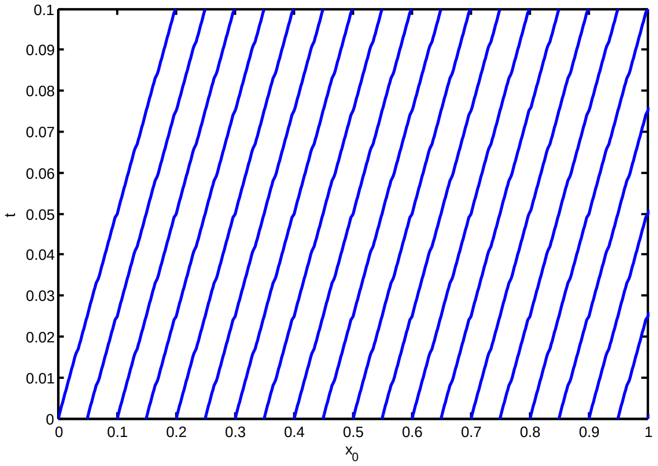

Figure 1: Trajectory lines

The constant x_{0i} in solution (41) indicates the origin positions of the particles on the x axis; where by the values of the concentration (initial condition) are assigned initially. For a small time interval Δt the particles moved foward to the another new positions $x(\Delta t)$ along the x-t plane with their concentration. Meanwhile, the concentration of the component remains unchanged during the movement of the particle along characteristic curves. The new positions of the particles along the characteristic curves become the solution of the convective subproblem of the model. This property plays the main roles in the construction of all Lagrangian and semi-Lagrangian algorithms for convective transport. Next, the solution or result of the convection subproblem is passed through the reaction subproblem where it is used as an initial condition according to the algorithm stated in chapter three. For a time step Δt, this can be done as follows; using the idea of Lagrangian coordinates, the equation (34) is reduced to a total time derivative and solved under the framework of operator splitting approach.

$$\frac{dC}{dt} = \frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} = D\frac{\partial^2 C}{\partial x^2} + f(x,t,C) \tag{42}$$

$$\frac{dC}{dt} = f(x,t,C) \tag{43}$$

Recall that $f(x,t,C) = kC_i$, then

$$\frac{dC_i}{dt} = kC_i \qquad i = 1,2,3,\cdots,n. \tag{44}$$

By integrating equation (44) gives the solution of reaction subproblem at particle i and is given by;

$$\int_{C_0}^{C_i(t)} \frac{dC_i}{C_i} = \int_{t_0}^{t} kdt \tag{45}$$

$$C_i(t) = C_0 exp(k(t-t_0)) \tag{46}$$

Hence, the integration should be done in each grid point at a small time step Δt along the computational domain. In the computation, Runge-Kutta has used to integrate the equation (44) by using MATLAB 7.3.0 (R2007a) on 2x3GHz Dual Core Xenon 8Gb desktop PC. The diffusion subproblem extracted from equation (34) can be solved in different numerical methods. Finite difference method and finite element method leads to a similar formulation of the problem and they are both efficient and stable for a pure diffusion problem [10]. Then, finite difference method has been used to discretize the second derivative in spatial (4^{th} - order space discretization) for the approximation of the solution and it has given as follows. Fisrt, the number of grid points N in the computational domain including the boundary points should be given. Second, the lower boundary value of xl should be given. Third, the upper boundary value of xu should be given and fourth, the value of the dependent variable $C(x_i)$ at each grid point x_i should be known. Then, from equation (47) the diffusion subproblem is stated as;

$$\frac{dC}{dt} = D\frac{\partial^2 C}{\partial x^2} \tag{47}$$

where the second derivative is computed by the central five point scheme using the function DSS044. The value of the component or function at each node or grid point

i, for small time interval Δt obtained after integrating the system of equations (44) by either Runge-Kutta method or Euler method (ODE solvers). Furthermore, the solution of this part becomes the solution to the general equation (34) for a time step Δt. In fact, at each time step;

(i) the whole component in the system is moved toward the output according to convective velocity,

(ii) a reaction occurs according to the reaction rates at each location in the computational domain,

(iii) diffusion occurs throughout the system,

Then, the different solutions of an equation (34) are simulated and shown in the Figures $5, 10$ using PTM and the method of lines (MOL), both based on the 4^{th}-order space discretization. In figure 5, the PTM technique has introduced 17 particles in the steep fronts of the initial condition and reaction solution using both adaptivities with $N_{max} = 5$. The uniform grid with 50 nodes have used to compute the diffusion subproblem. In case of computation time, CPU has taken 3.91seconds to execute 21 time steps using PTM, while 0.51 seconds have used to execute the same problem using MOL. In Figure 10 with inflow condition 19 particles have introduced in the vicinities of the singularities of initial condition, inflow condition and reaction solution when PTM applied.

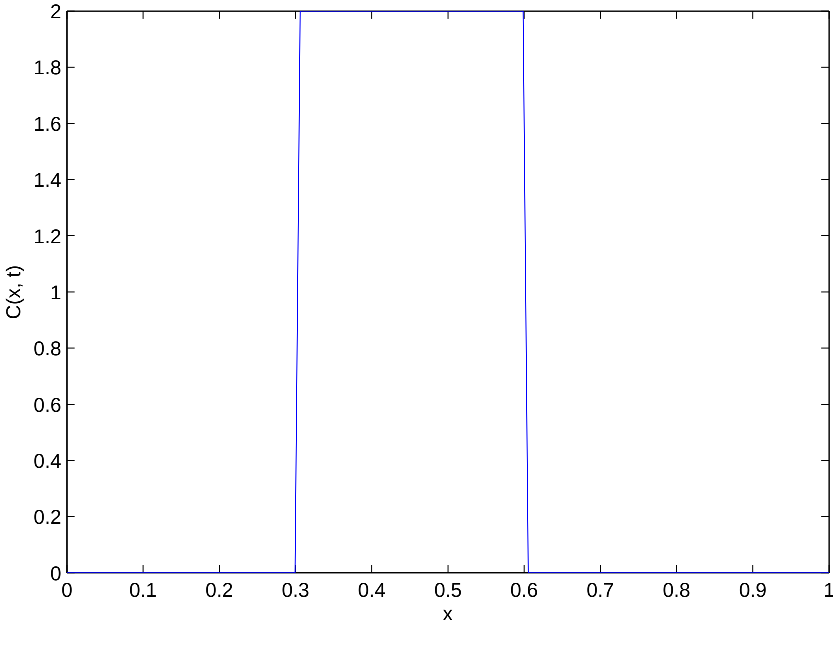

Figure 2: Initial distribution of step - function

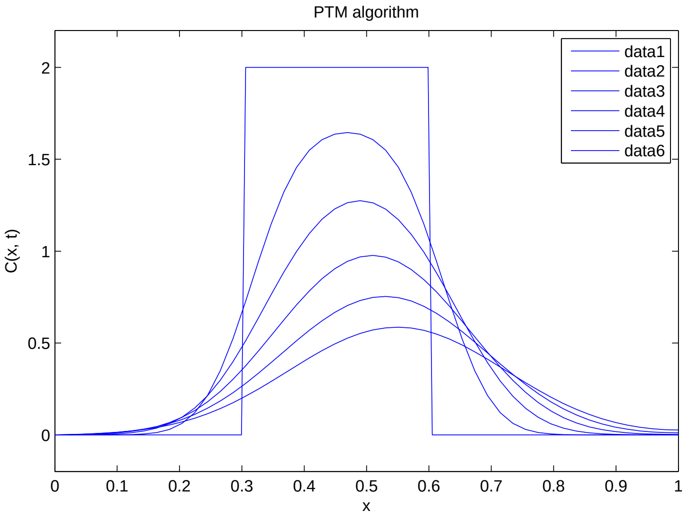

Figure 3: Solutions of convection diffusion reaction problem simulated by PTM at $t = 0.02, 0.04, 0.06, 0.08$ and 0.10 without inflow condition

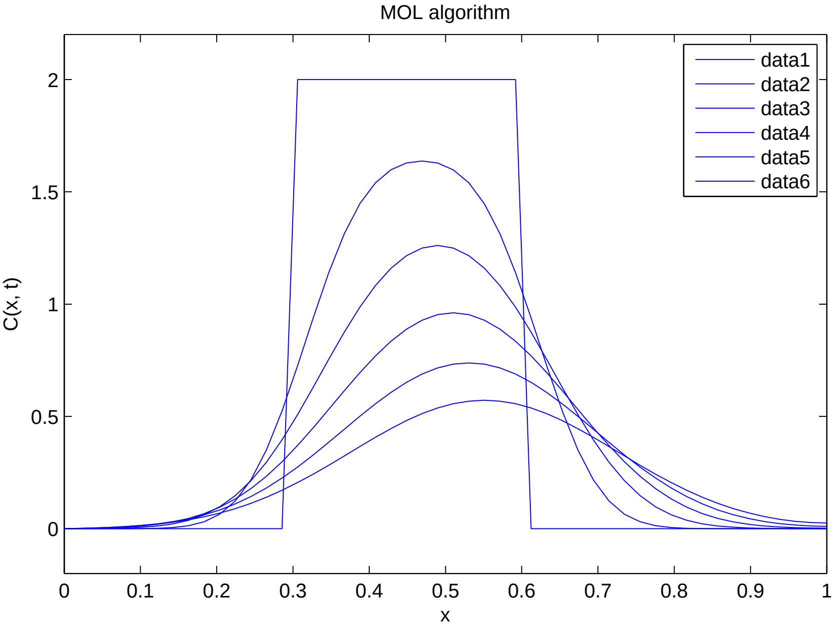

Figure 4: Solutions of convection diffusion reaction problem simulated by MOL at $t = 0.02, 0.04, 0.06, 0.08$ and 0.10 without inflow condition

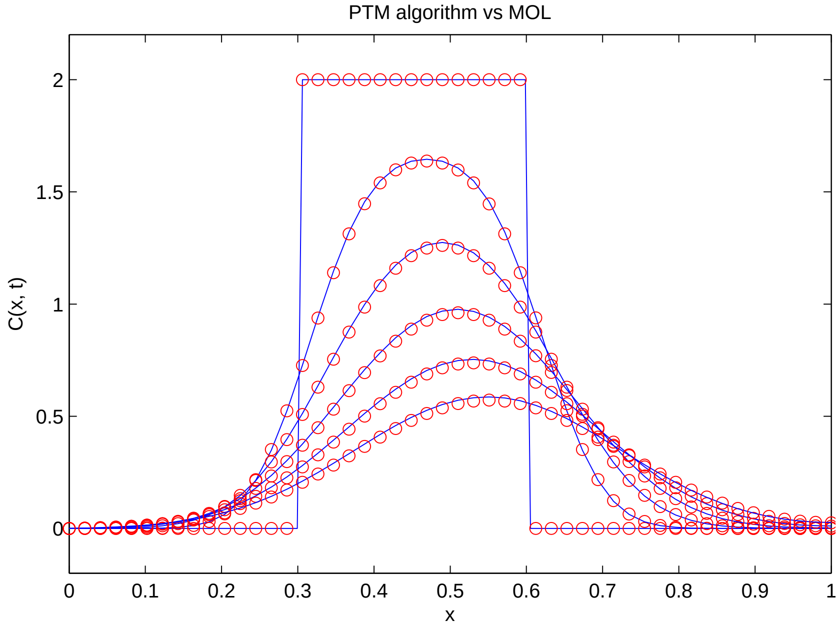

Figure 5: Solutions of CDR problem obtained by PTM (the solid line) and MOL (the circles) with no inflow condition at $t = 0.02, 0.04, 0.06, 0.08$ and 0.10

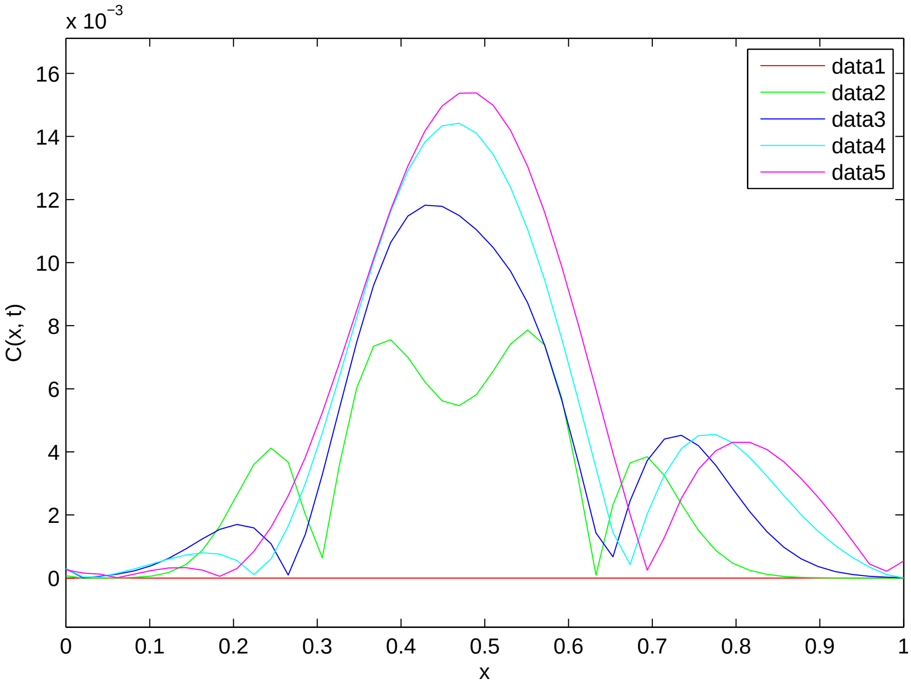

Figure 6: Deviation of solutions between PTM and MOL after 4 simulations

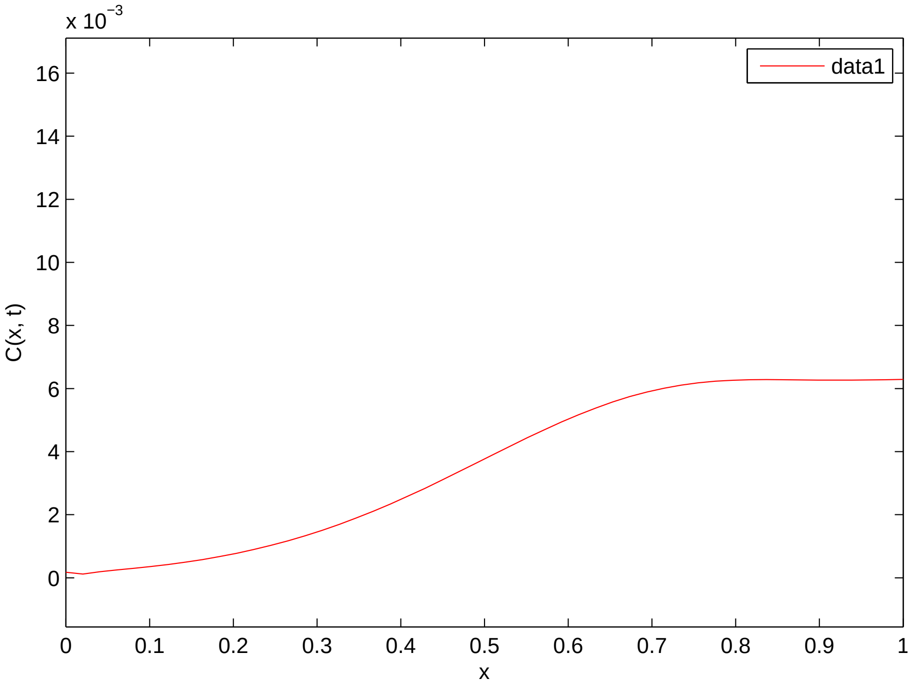

Figure 7: Deviation of two solutions at $t = 4.2$

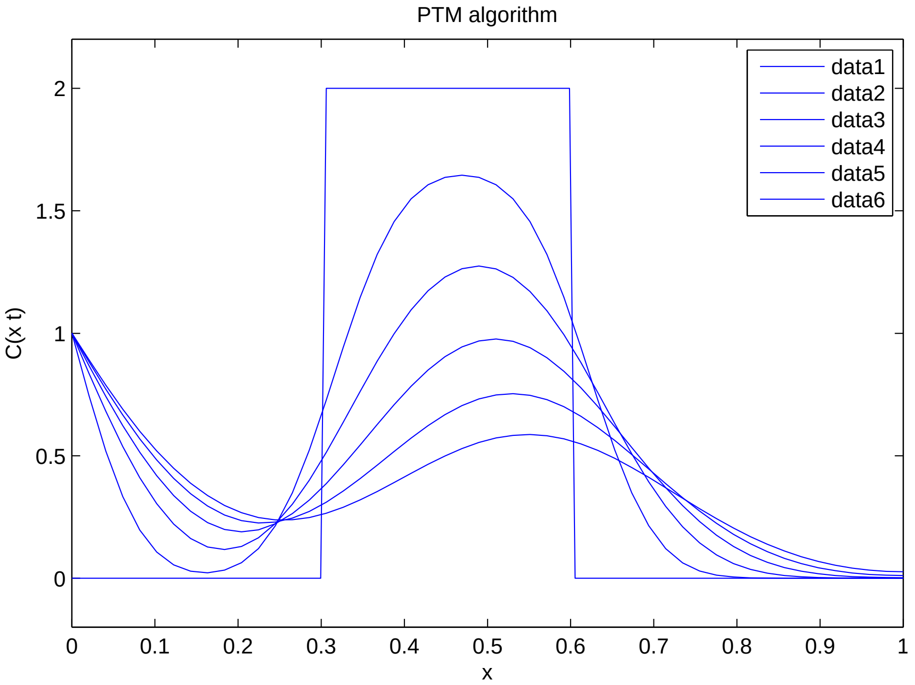

Figure 8: PTM with inflow condition simulated at $t = 0.02, 0.04, 0, 06, 0.08$ and 0.10

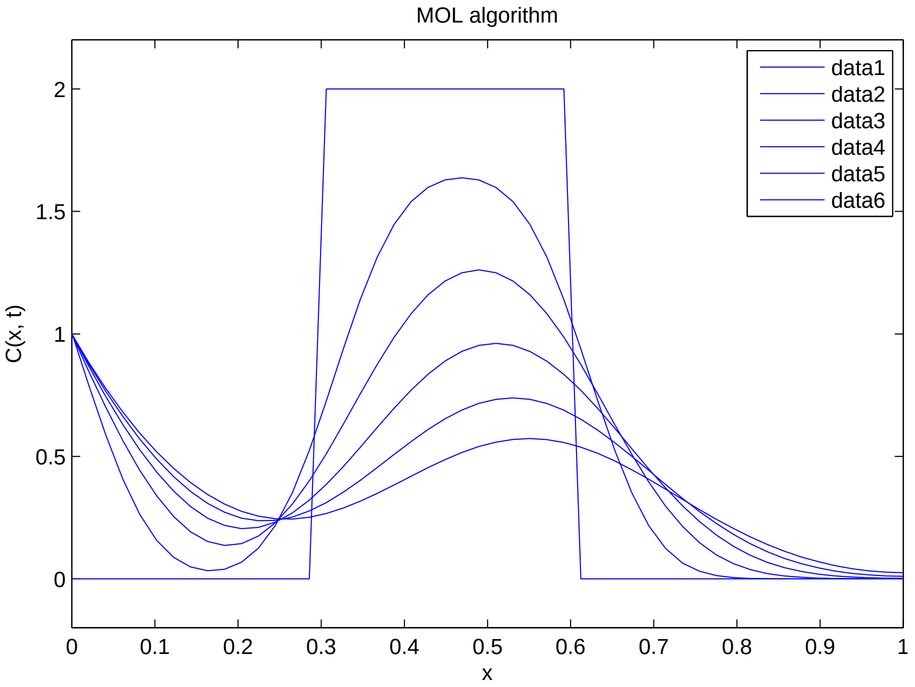

Figure 9: MOL with inflow condition simulated at $t = 0.02, 0.04, 0.06, 0.08$ and 0.10

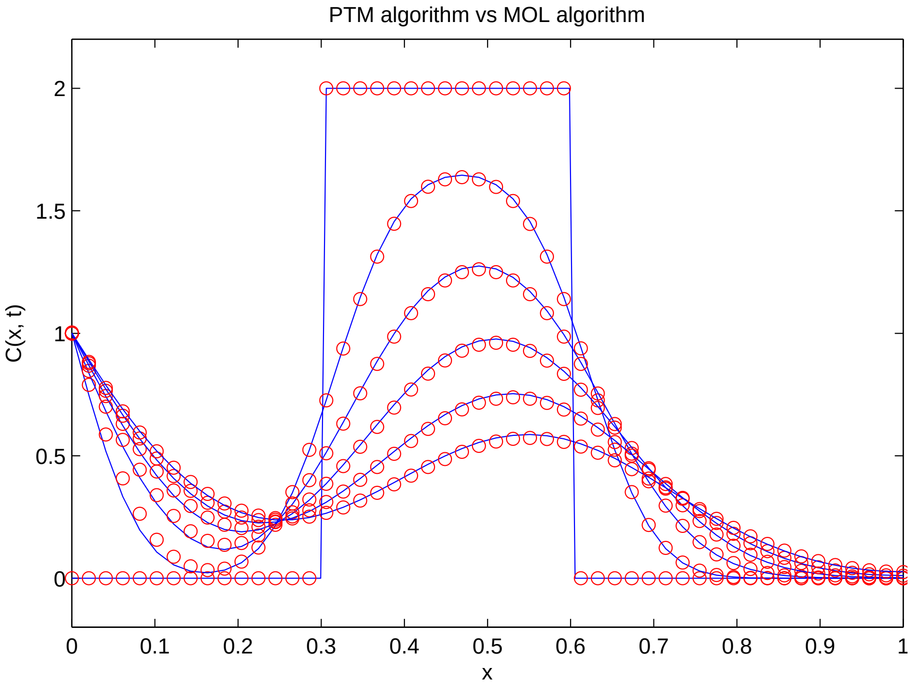

Figure 10: PTM (the solid line) and MOL (the circles) with inflow condition after $t = 0.02, 0.04, 0.06, 0.08$ and 0.10

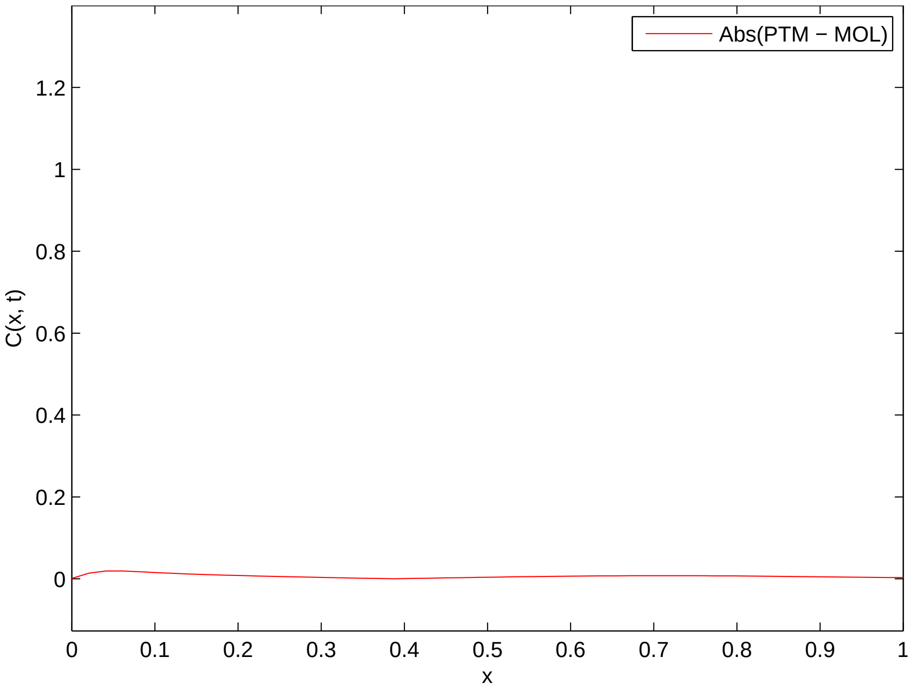

Figure 11: Deviation of two solutions at step 21

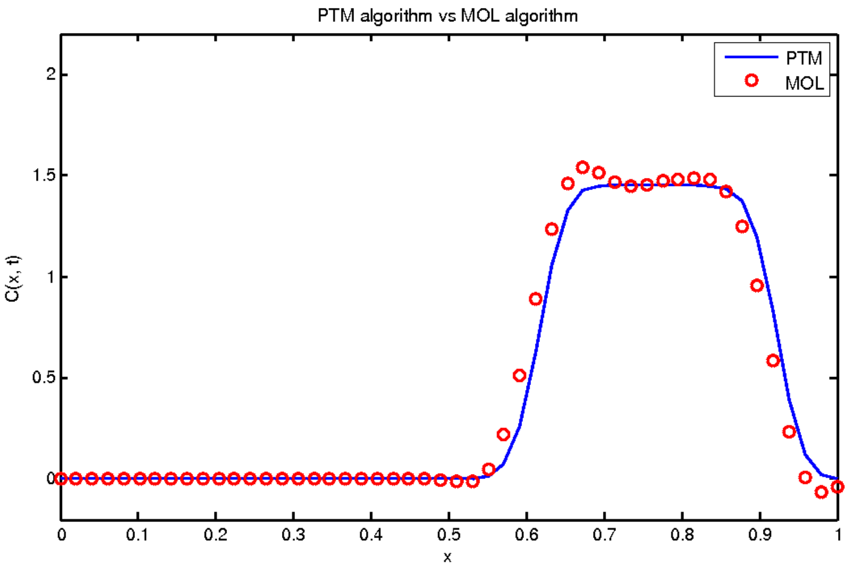

Figure 12: Convection diffusion reaction of the step-function, $D = 0.001$; the line- the numerical solution obtained by PTM and the circles- the numerical solution obtained by MOL at $t = 4.2$

To accomplish an error analysis, the goal of the simulation is to test the performance of the new technique and to compare its solutions with solutions of MOL. Figures $5, 10$ have computed by PTM technique and MOL technique respectively, together

with the solution of Figure 23 simulated at $t = 4.2$. To estimate the order of the method's accuracy we measure the error in deviation form between two techniques at each grid point in every simulation;
$\left\|C^{PTM} - C^{MOL}\right\| = \|C^{ex} - C^{ap}\|$, where C^{ex} and C^{ap} are exact and approximated solution of the model, respectively.

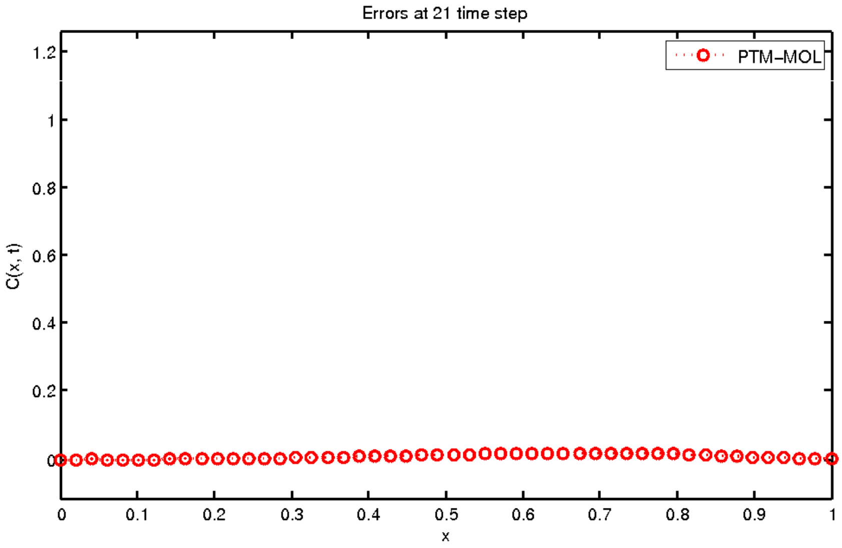

Figure 13: The plot of errors in table 2, computed from figure 12

The two Figures 5, 10 show almost the same characteristics or behavior of solutions simulated by PTM and MOL on the same grid for the whole convection diffusion reaction problem. In Figure 5, both methods produce almost similar results for each simulation with no inflow condition on the inlet. This implies that, deviation of two solutions at every grid point simulated by PTM and MOL is very small in magnitude (table 2). However, in Figure 10 with inflow condition, the solutions differ in large magnitude around the inflow portion but near the outflow the solutions are equal. On another hand, if D is small in the process the MOL produces artificial oscillations (non - physical features) especially in the steep fronts of initial condition and inflow condition. These unwanted oscillations or artificial oscillations are shown in Figure 12. Furthermore, PTM technique does not suffer from the strength of the two terms (convection and diffusion) in the system, while MOL with small diffusion coefficient is not suitable for simulation of CDR problem. In Figures 6, 7, 11 and 13 show some deviations of solutions simulated by two techniques at different time steps along the computational domain. In general, diffusion term smooth the final solution by removing all the non-physical oscillations on the vicinities of the final solution and leads to the improvement of the solution at each time step.

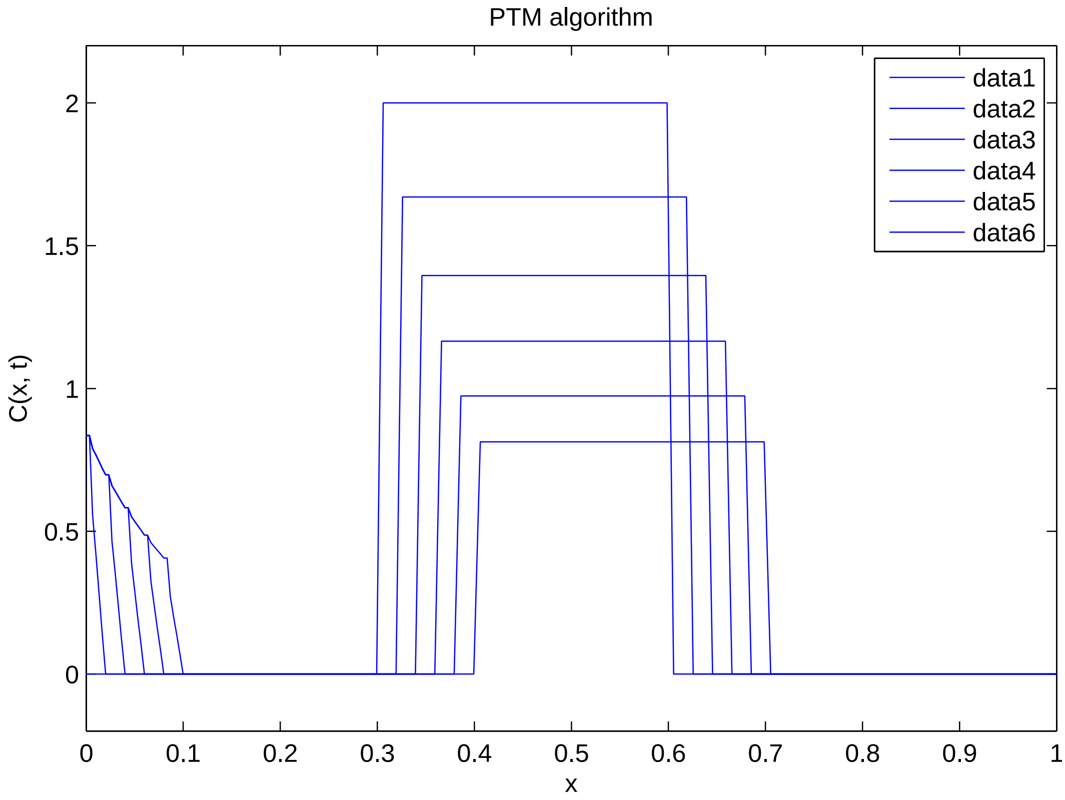

Figure 14: PTM with $D = 0$

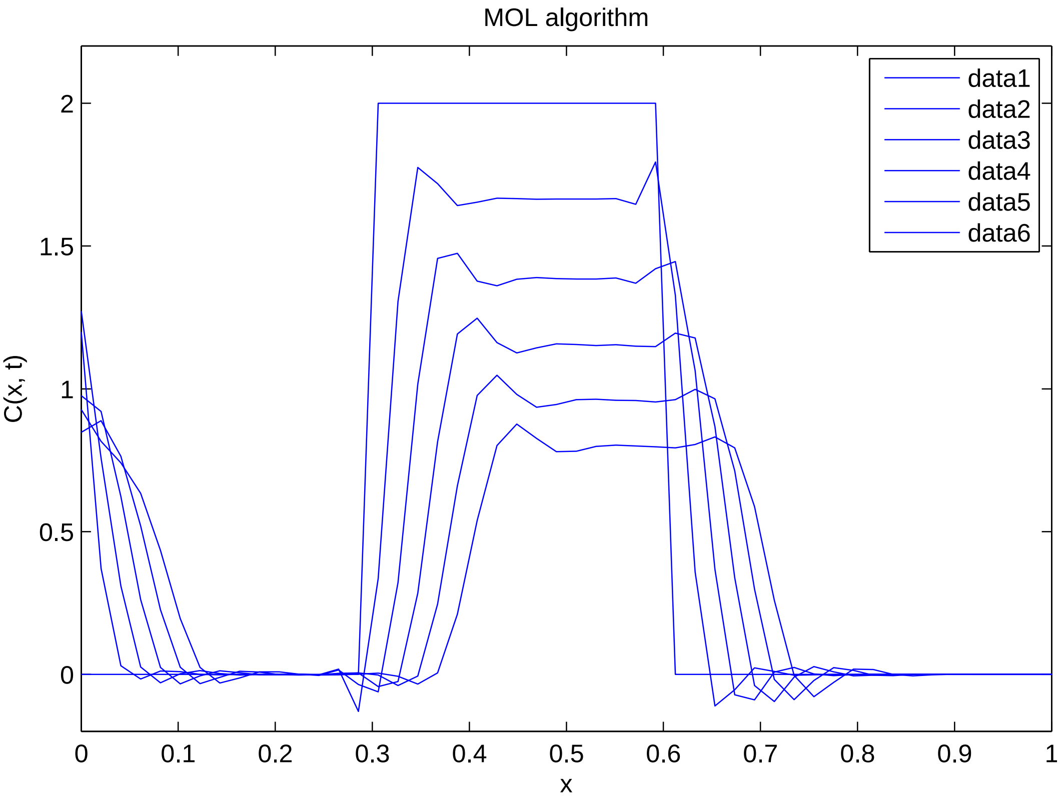

Figure 15: MOL with $D = 0$

Furthermore, MOL produces worse approximated solution to the model especially when $D = 0$ (large oscillations) as shown in Figure 15. Meanwhile, the PTM controls these oscillations at the steep fronts of the approximated solution (Figure 14). Hence, the PTM produces an accurate solution of the model regardless the value of D is very small. At large D, both techniques remove these spurious oscillations in the steep fronts of the approximated solution. In Figures 14 - 15, data1 = initial condition, data2 = simulation 1, data3 = simulation 2, data4 = simulation 3 and data5 = simulation 4.

4.2 Non-stiff multicomponent reactive transport model

In the previous section (section 4.1) we have solved numerically (particle transport method) the equation that model the flow of one component along one direction. The solution of the model has been compared with the method of line which is also a numerical approximation approach. Then, for the next section the same approach is applied to nonstiff chemical kinetics with three components advected through the computational domain with a constant velocity field u. The model considered here is convection dominated problem with small diffusion coefficient. For a one dimensional multicomponent reactive flow through homogeneneous medium is given in two forms. The first part denotes interaction of elements equation (48) and the second part combined both processes equation (49). The transport modeling equation (49) leads to second order partial derivatives of a non-linear differential equations in $[a, b] \times [0, T]$;

$$C_1 + C_2 \xrightarrow{k} C_3 \tag{48}$$

$$\begin{aligned} \frac{\partial C_1}{\partial t} + u\frac{\partial C_1}{\partial t} &= D\frac{\partial^2 C_1}{\partial x^2} - kC_1C_2 \\ \frac{\partial C_2}{\partial t} + u\frac{\partial C_2}{\partial t} &= D\frac{\partial^2 C_2}{\partial x^2} - kC_1C_2 \\ \frac{\partial C_3}{\partial t} + u\frac{\partial C_3}{\partial t} &= D\frac{\partial^2 C_3}{\partial x^2} + kC_1C_2. \end{aligned} \tag{49}$$

The model (49) is associated with initial conditions and boundary conditions as well. The initial conditions of the model and their distributions along the domain $[a, b]$ are given as shown below ;

$$C_1(x, 0) = \begin{cases} 1 & \text{if } 0.3 <= x <= 0.6 \\ 0 & \text{otherwise} \end{cases} \tag{50}$$

$$C_2(x, 0) = \begin{cases} 2 & \text{if } 0.3 <= x <= 0.6 \\ 0 & \text{otherwise} \end{cases} \tag{51}$$

$$C_3(x, 0) = \begin{cases} 0.7 & \text{if } 0.3 <= x <= 0.6 \\ 0 & \text{otherwise} \end{cases} \tag{52}$$

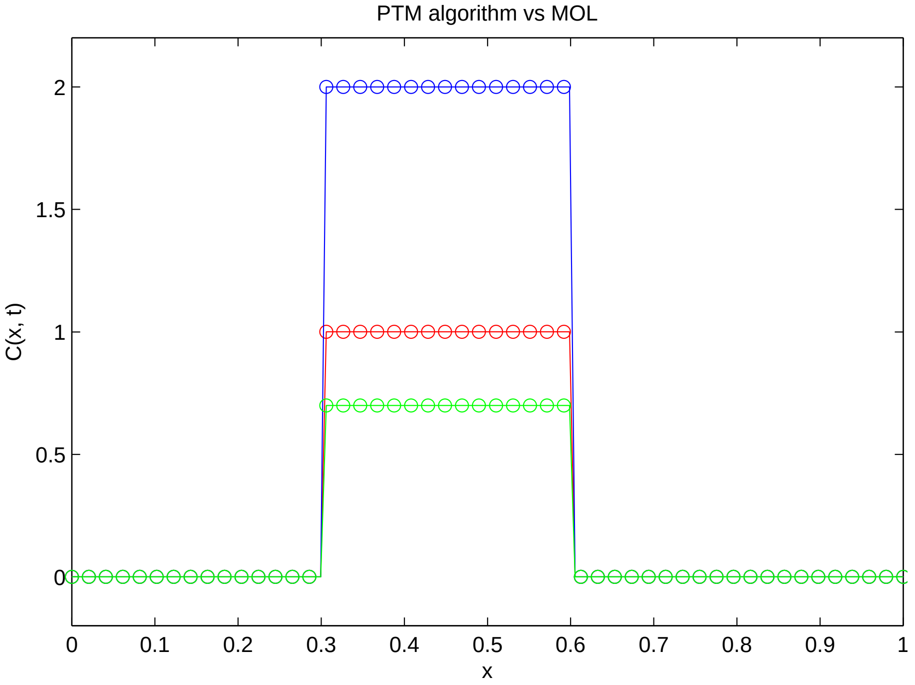

Figure 16: Initial distribution of the concentrations in the domain

The inflow and outflow conditions on $[a, t]$ and $[b, t]$ respectively are also provided below;

$$C_1(0,t) = 1; C_2(0,t) = 2; C_3(0,t) = 0.7 \tag{53}$$

$$\frac{\partial C_1(L,t)}{\partial x} = \frac{\partial C_2(L,t)}{\partial x} = \frac{\partial C_3(L,t)}{\partial x} = 0 \tag{54}$$

given that C_1, C_2 and C_3 are the concentrations of each reactant and D, the diffusion or dispersion coefficient. In this work, D is assumed to be the same for all species and constant number (arbitrary number). The source terms, $-kC_1C_2$ and kC_1C_2 depend on the reaction rate constant k and the reaction concentrations. Furthermore, u is a transport or convective velocity and is also assumed to be the same along the computational domain. The source terms in equation (49) are derived from the bimolecular reaction in the system that has the form given in equation (48); meaning that C_1 and C_2 interact within the system as a result C_3 is created at a rate k per unit time. Given that;

$$f(x, t, C_1) = -kC_1C_2$$

$$f(x,t,C_2) = -kC_1C_2$$
$$f(x,t,C_3) = +kC_1C_2.$$

The three terms in the right hand side of these equations represent the function $f(x,t,C_i)$ of the equation (49) as the source or sink terms of the coupled system. Reaction rate constant k used in reactive transport modeling is usually determined in bath experiment where the reactants are well homogenized. But in this work an arbitrary reaction rate k is used without conducting any experiment setup. The diffusion coefficient D used as the homogenizer of the reactants within the system (Kapoor *et al 1997, 1998*). Equation (49) is divided into three parts under the framework of operator splitting approach for computation along the domain $[a,b]$. Both adaptivities have applied at the initial stage and inflow stage because, they balance between high resolution of singularities and small computational costs. In general, adaptivity procedure used to densifying the particle system, in the regions where initially there were few nodes or particles. Thus, after densifying these particles set along the computational domain $[a,b]$, then the characteristic curves (or trajectories) which are defined by ordinary differential equation (55) can be solved;

$$\frac{dx}{dt} = u(x,t) \tag{55}$$

On the other hand, characteristic curve satisfies the ordinary differential equation (55) as a solution and originates from the initial particle position. These curves allow the particles to move along them with the concentrations or reactants initial distributed in the computational domain at a small time step Δt. Moreover, each particle along the characteristic curve carries the physical quantities (concentrations) involved at the processes in the domain $[a,b]$. This indicates that, the convective transport of the solution as well as integration of the reaction terms are carried out by the particles. Apart from that, stationary mesh in the domain and a moving system of particles should be implemented for the achievement of better approximated solution. Then, equation (49) is decoupled into two subproblems at each time interval $[t_{m-1}, t_m], m = 1, 2, \cdots M$ on $[0,T]$ as stated below.

(i) Convection reaction subproblem

$$\begin{aligned}\frac{\partial C_1}{\partial t} + u\frac{\partial C_1}{\partial t} &= -kC_1C_2\\ \frac{\partial C_2}{\partial t} + u\frac{\partial C_2}{\partial t} &= -kC_1C_2\\ \frac{\partial C_3}{\partial t} + u\frac{\partial C_3}{\partial t} &= +kC_1C_2\end{aligned} \tag{56}$$

$$C_i(x,t) = C^{m-1}(x) \tag{57}$$

$$C_i(0,t) = C_{in}(t). \tag{58}$$

Since the technique uses Lagrangian coordinates approach, an equation (56) is reduced to a total time derivative and is equal to the reaction term in the model with three cases. Furthermore, convection reaction subproblem becomes;

$$\begin{aligned}\frac{dC_1}{dt} = \frac{\partial C_1}{\partial t} + u\frac{\partial C_1}{\partial t} &= -kC_1C_2\\ \frac{dC_2}{dt} = \frac{\partial C_2}{\partial t} + u\frac{\partial C_2}{\partial t} &= -kC_1C_2\\ \frac{dC_3}{dt} = \frac{\partial C_3}{\partial t} + u\frac{\partial C_3}{\partial t} &= +kC_1C_2.\end{aligned} \tag{59}$$

Equation (59) is simplified further and becomes;

$$\begin{aligned}\frac{dC_1}{dt} &= -kC_1C_2\\ \frac{dC_2}{dt} &= -kC_1C_2\\ \frac{dC_3}{dt} &= kC_1C_2.\end{aligned} \tag{60}$$

As stated in the methodology section, the solution of this subproblem (60) $C^{**}(x,t)$ defines the initial condition of the diffusion subproblem. We simulated the problem on the time interval $[0, 4.2]$ with the time step $\Delta t = 0.02$, convective velocity $u = 0.1$ and kinetic reaction $k = 0.5$ on the domain $[0, 1]$. For $D = 0$, solutions of convection reaction subproblem at $t = 4.2$ are computed with particle transport method technique Figure 17 and method of lines Figure 18.

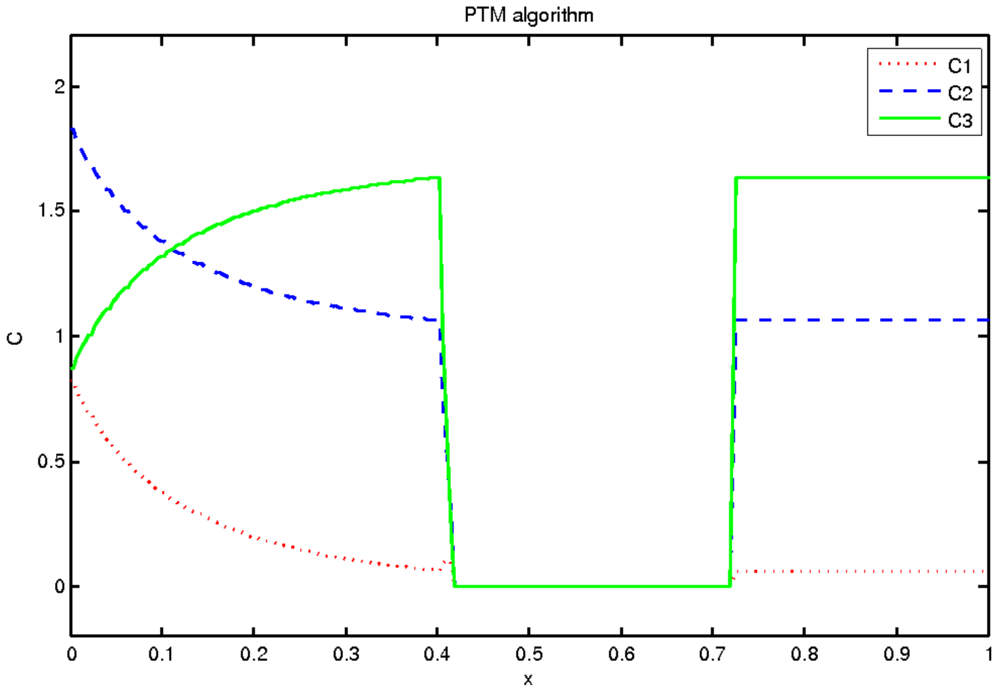

Figure 17: Three step-functions transport with reaction process simulated by PTM at t = 4.2

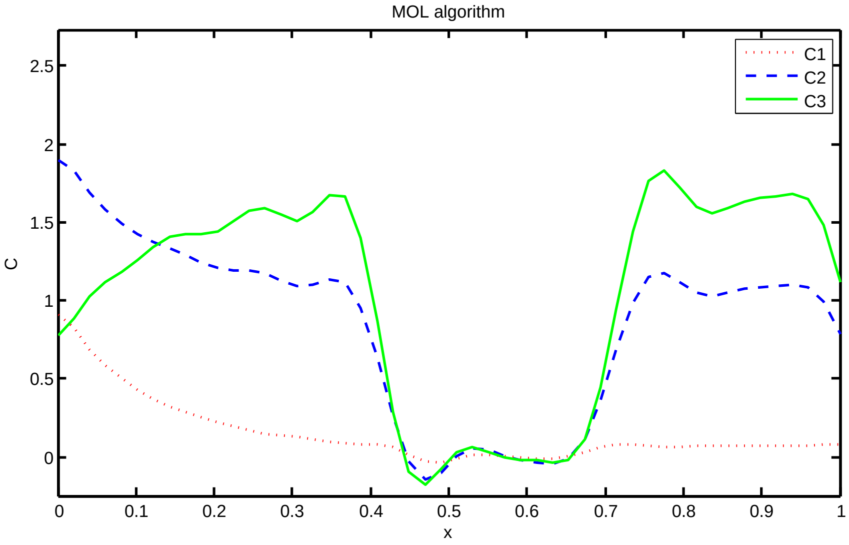

Figure 18: Three step-functions transport with reaction process simulated by MOL at t = 4.2

In the case of PTM technique, initially 26 particles are distributed randomly on $[a, b]$. After initial adaptivity with $N_{max} = 5$ the system of particles increase up to 36 particles. Ten additional points or particles are introduced in the vicinity of discontinuities. In Figure (17), inflow adaptivity and solution dependent adaptivity add more particles on the inflow portion of the domain and in the domain respectively. The added particles make the solution of the model to increase its resolution, especially on the discontinuity parts. But in Figure (18) such kind of adaptivities are not included in the simulation process, then, the final solution always possess some artificial oscillations on the steep fronts or the region with high gradient value. These features limit the applicability of this method (MOL) for the non - diffusivity problem. By considering the diffusion coefficient to be non-zero value, projection technique has used to project the particle set onto the uniform grids (50 stationary grids have used). The projection technique as explained to the methodology part, is based on the linear interpolation between two nearest particles for each stationary grid. Using the subsolution $C^{**}(x,t)$ of convection reaction subproblem, the final solution of the whole system has simulated with $D = 0.01$ in the domain of stationary grids. In figure 19, the approximated solutions simulated by PTM technique between $t = 0 - 0.1$ are plotted on the same axis, while in Figure 20 MOL is applied to solve the same problem on the same grid points, using the same duration of the computation. The two solutions are almost similar but in figure 20, the initial conditions are not exact steep because they have not sitted on the particles. Figure 21, shows the solution at $t = 3$ using PTM and MOL and both of them show the same behavior, but in the inflow part the solutions tend to deviate at the small amount. The all information (solutions) are stored in the grid point within the computational domain.

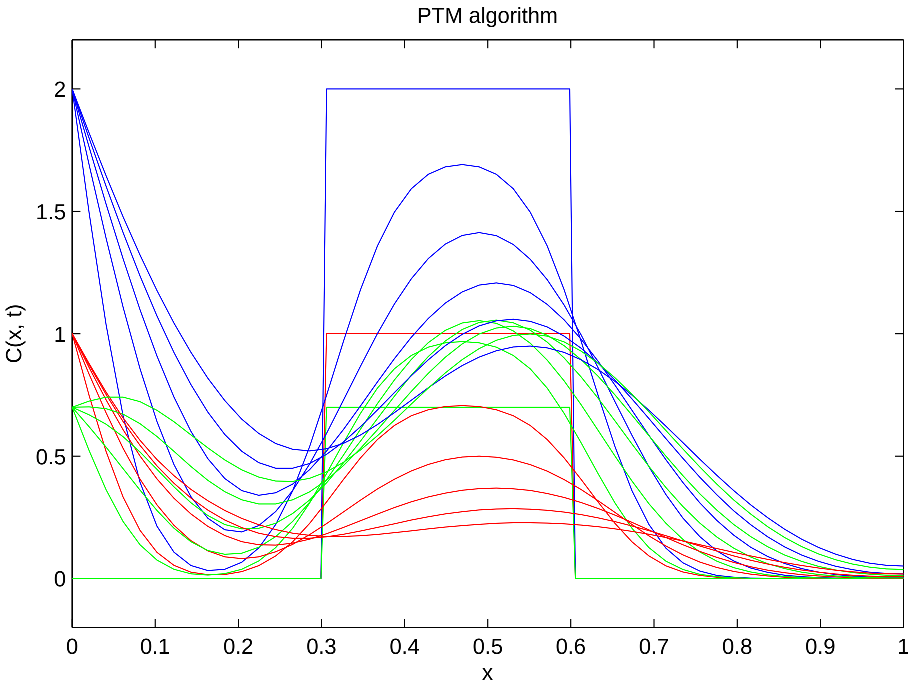

Figure 19: Simulation of nonstiff chemical kinetics by PTM; $D = 0.01$ at different time steps

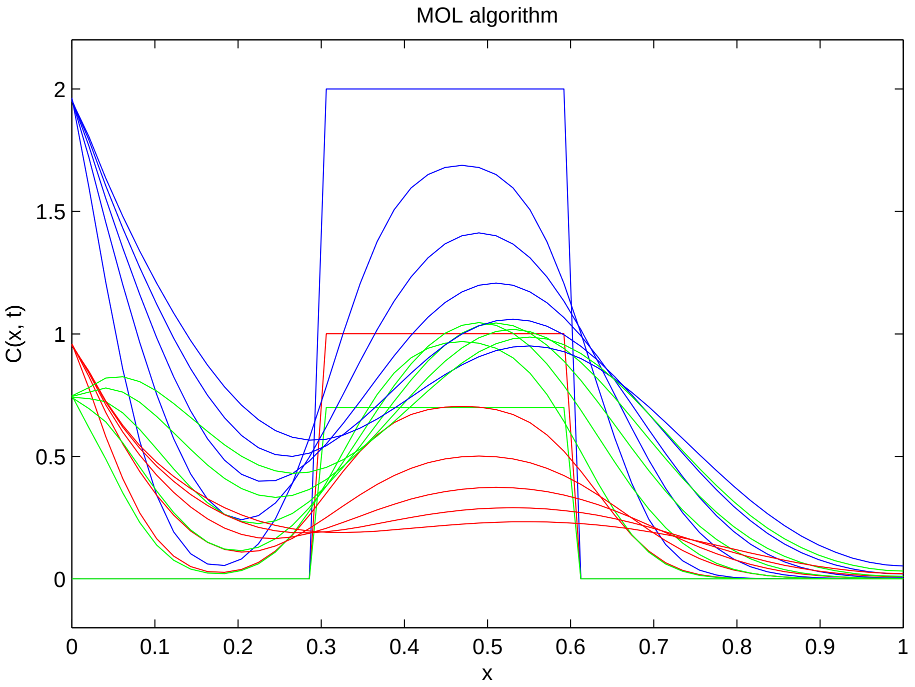

Figure 20: Simulation of nonstiff chemical kinetics by MOL; $D = 0.01$ at different time steps

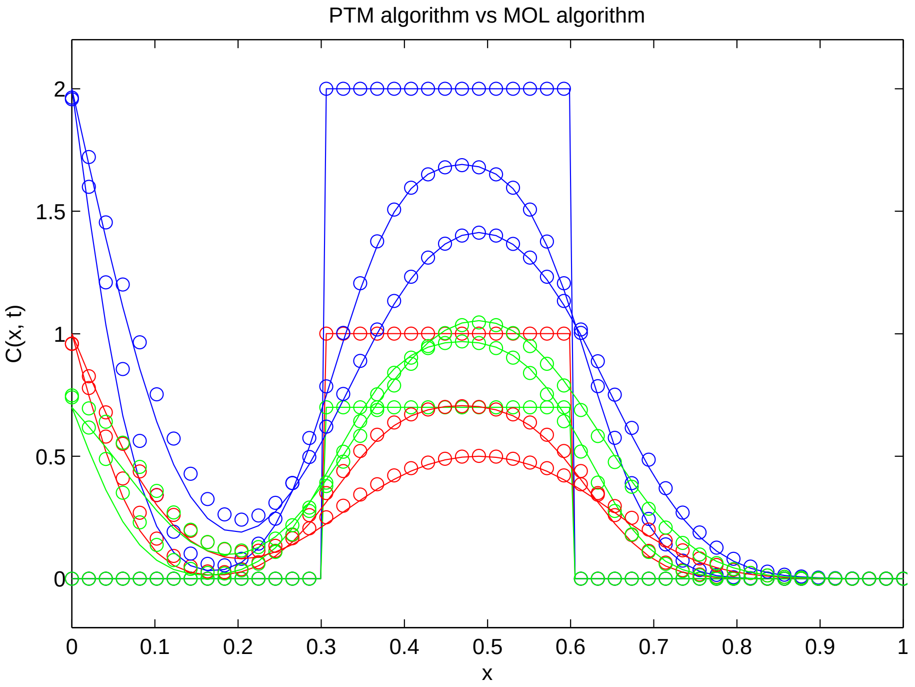

Figure 21: Convection diffusion reaction simulation, $D = 0.01$; the solid line - the numerical solution obtained by PTM and the circles - the numerical solution obtained by MOL, at $t = 0.02, 0.04, 0.06, 0.08$ and 0.10

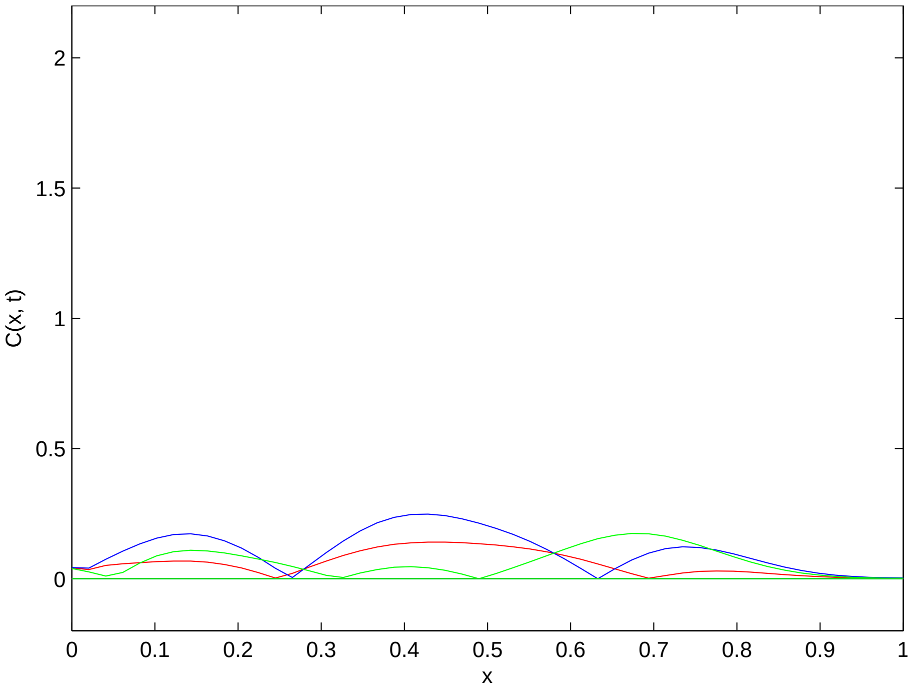

Figure 22: Deviations (errors) distribution between 5 simulations

Figure 22, shows that at every grid point, the difference in solutions between the two techniques become large if the grid is allocated at the steep front of an approximated solution.

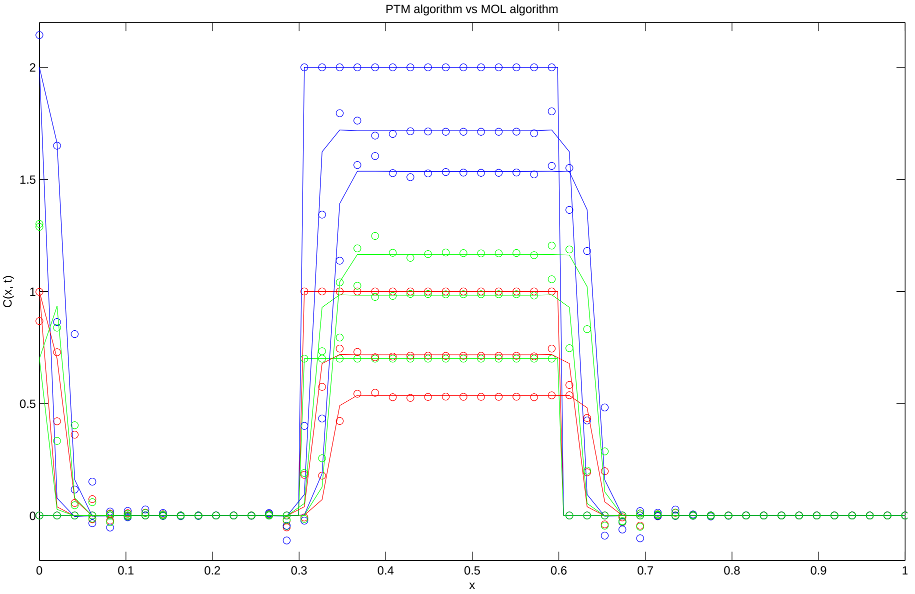

Figure 23: Convection diffusion reaction simulation, $D = 0.0001$; the solid line - the numerical solution obtained by PTM and the circles - the numerical solution obtained by MOL, at $t = 0.02, 0.04$

In figure 23, the approximated solutions are simulated by both techniques between $t = 0.02 - 0.04$ and plotted on the same axis. The numerical solutions simulated by MOL tend to oscillate below x - axis (negative concentrations). These features are caused by the small diffusion coefficient on the model (small smoothing of the artificial oscillations). But for the large D using MOL, these features disappeared, due to the high rate of smoothing the simulated solution. PTM technique works properly for any change of these parameters of the model, but MOL often depends on the diffusion coefficient for the better results.

4.3 A stiff system (Ozone in the Atmosphere)

The method or technique that has presented in this thesis (Particle transport method) has been tested to the models of different nature, one model had only one component and the second model had three components with the same reaction rate along the computational domain. Finally, we have tested our technique on a stiff system which is based on the behaviour of ozone in the atmosphere with other gases. Usually, we call a system to be stiff if some of the elementary reactions be much faster than the others in their interaction. This behaviour causes the system to have big and small numbers of reaction rates and becomes difficulty to simulate the model in every time step [30]. Moreover, this section describes one such problem concerning about the modeling of the amount of ozone in the atmosphere. For more information about modeling of ozone in the atmoshere read the paper by Hindmarsh (1980) or [23]. At high altitude ozone protects us from most of the sun's harmful ultraviolet radiation, and some scientists feel that the release of CFLs (Chlorofluorocarbons) gases and associated pollution are causing permanent changes in its level. For us, the model illustrates the kind of stiff initial boundary value problem that will be simulated by using MATLAB 7.3.0$(R2007a)$ on $2x3GHz$ Dual Core Xenon $8Gb$ desktop PC. As an example, we study a model for ozone in atmosphere. We assume that the earth's atmosphere is a closed system held at a constant temperature and volume and let us consider the simultaneous interaction of three chemicals, free oxygen O, ozone O_3, and molecular oxygen O_2 in the system. One reaction mechanism for these chemicals is;

$$\begin{aligned} O + O_2 &\overset{k_1}{\to} O_3 \\ O + O_3 &\overset{k_2}{\to} 2O_2 \\ O_2 &\overset{k_3(t)}{\to} 2O \\ O_3 &\overset{k_4(t)}{\to} O + O_2 \end{aligned} \tag{61}$$

The reaction tells that the equations for O and O_2, O and O_3, O_2 and O_3 respectively must include loss terms, because the concentrations of these are being reduced by the reaction. Similarly the equations for O_3, $2O_2$, $2O$ and $O+O_2$ involve production or gain term. The loss or gain is defined as the product of the concentration of the two losing chemicals and the rate constant. In our model, the notation $k_3(t)$ and $k_4(t)$ means that the rate constants change with time. This is because the last two reactions describe the effect of sunlight, which causes molecular oxygen O_2 and ozone O_3 to photodissociate. In this work the model will be assumed to vary its concentrations with altitude, due to the movement of concentrations or gases caused by wind. Furthermore, the model described above can be deduced into the system of differential equations as shown below;

$$\begin{aligned} \frac{d[O]}{dt} &= -k_1[O][O_2] - k_2[O][O_3] + 2k_3(t)[O_2] + k_4(t)[O_3] \\ \frac{d[O_2]}{dt} &= 0 \\ \frac{d[O_3]}{dt} &= k_1[O][O_2] - k_2[O][O_3] - k_4(t)[O_3] \end{aligned} \tag{62}$$

The initial conditions together with the boundary conditions at the inflow part of the domain of these gases are given as follows;

$$O(x,0) = \begin{cases} 10^6 cm^{-cm} & \text{if } 0.3 <= x <= 0.6 \\ 0 & \text{otherwise} \end{cases} \tag{63}$$

$$O_2(x,0) = \begin{cases} 3.7 \times 10^{16} cm^{-1} & \text{if } 0.3 <= x <= 0.6 \\ 0 & \text{otherwise} \end{cases} \tag{64}$$

$$O_3(x,0) = \begin{cases} 10^{12} cm^{-1} & \text{if } 0.3 <= x <= 0.6 \\ 0 & \text{otherwise} \end{cases} \tag{65}$$

$$O(0,t) = 10^6 cm^{-1} \tag{66}$$

$$O_2(0,t) = 3.7 \times 10^{16} cm^{-1} \tag{67}$$

$$O_3(0,t) = 10^6 cm^{-1}. \tag{68}$$

The initial distribution of gases along the computational domain on the particle set are also shown in the Figures below;

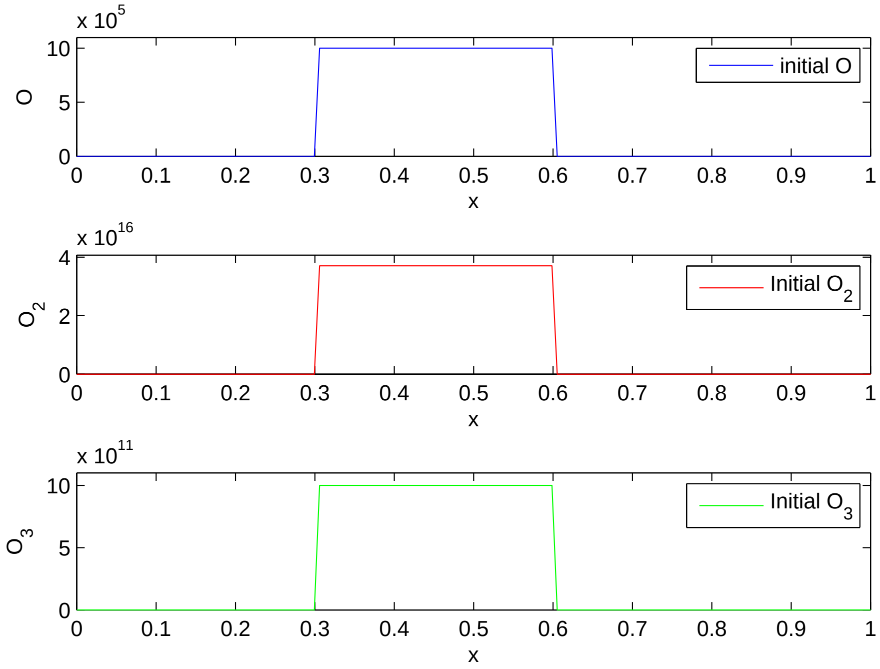

Figure 24: Three gases on the particle set

Since $[O_2]$ is many order of magnitude larger than $[O]$ and $[O_3]$ we assume that it is essentially unaffected by the other two and hence is constant for all time. Therefore we can ignore its differential equation. The rate constants k_1 , k_2 are known to be $k_1 = 1.63 \times 10^{-16}$, $k_2 = 4.66 \times 10^{-16}$, where the other two rate constants vary twice a day, and are modeled by

$$k_i(t) = \begin{cases} exp(-c_i/sin(wt)) & \text{if } \ sin(wt) > 0, \qquad i = 3, 4 \\ 0 & \text{if } sin(wt) < 0 \end{cases} \tag{69}$$

with $w = \pi/43200 second^{-1}$, $c_3 = 22.62$, $c_4 = 7.601$. The values of k_3 and k_4 rise rapidly beginning at dawn ($t = 0$), reach a peak at noon ($t = 6 \times 3600 seconds$), and decrease to zero at sunset ($t = 12 \times 3600 seconds$). Nevertheless, the model 61 indicates interaction of gases only (reaction) without an involvement of advection or diffusion in the system. Then an overall model that describes the three phenomena at every time step is stated as;

$$\begin{aligned}\frac{\partial O}{\partial t} + u_1\frac{\partial O}{\partial x} &= D_1\frac{\partial^2 O}{\partial x^2} + \frac{d[O]}{dt}\\ \frac{\partial O_2}{\partial t} + u_2\frac{\partial O_2}{\partial x} &= D_2\frac{\partial^2 O_2}{\partial x^2} + \frac{d[O_2]}{dt}\\ \frac{\partial O_3}{\partial t} + u_3\frac{\partial O_3}{\partial x} &= D_3\frac{\partial^2 O_3}{\partial x^2} + \frac{d[O_3]}{dt}\end{aligned} \tag{70}$$

We assume that due to the uniformity of the atmosphere and its motion,the value of some parameters should be considered to be the same i.e $D_1 = D_2 = D_3$ and $u_1 = u_2 = u_3$.

We simulated the model (70) using two approaches, the first approach (integration with stiff solver) has used by ignoring the other two processes (convection and diffusion) while the second method (particle transport method) has used by considering that the system is also affected by the motion of atmosphere as well as the diffusion of the components present in the system. Figures 25 − 27 show the simulated outcome concentrations of a system after two days ($48hrs$) of simulation using stiff solver (Runge - Kutta).

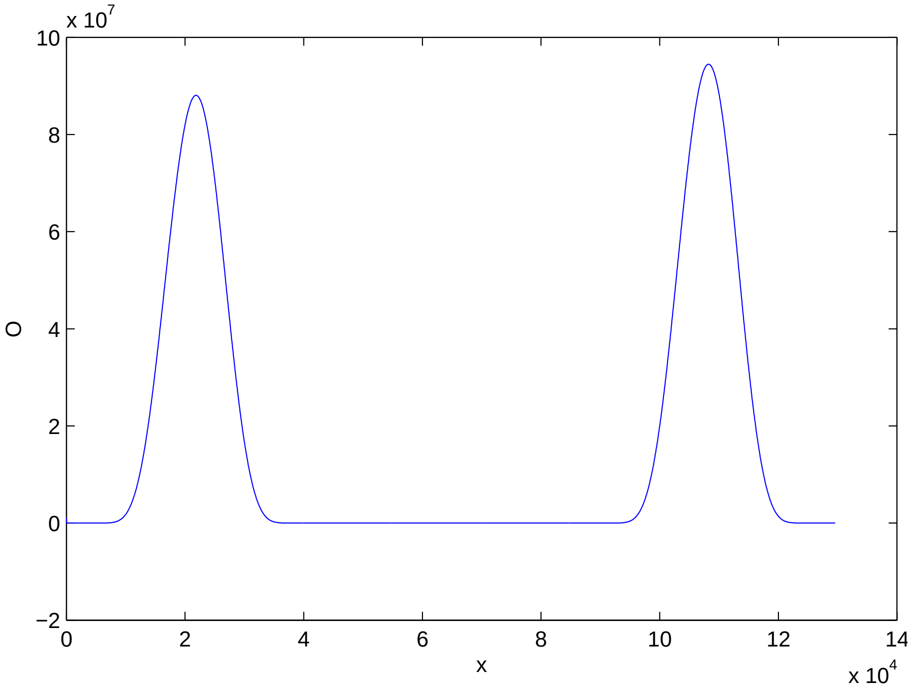

Figure 25: Free oxygen in the ozone model

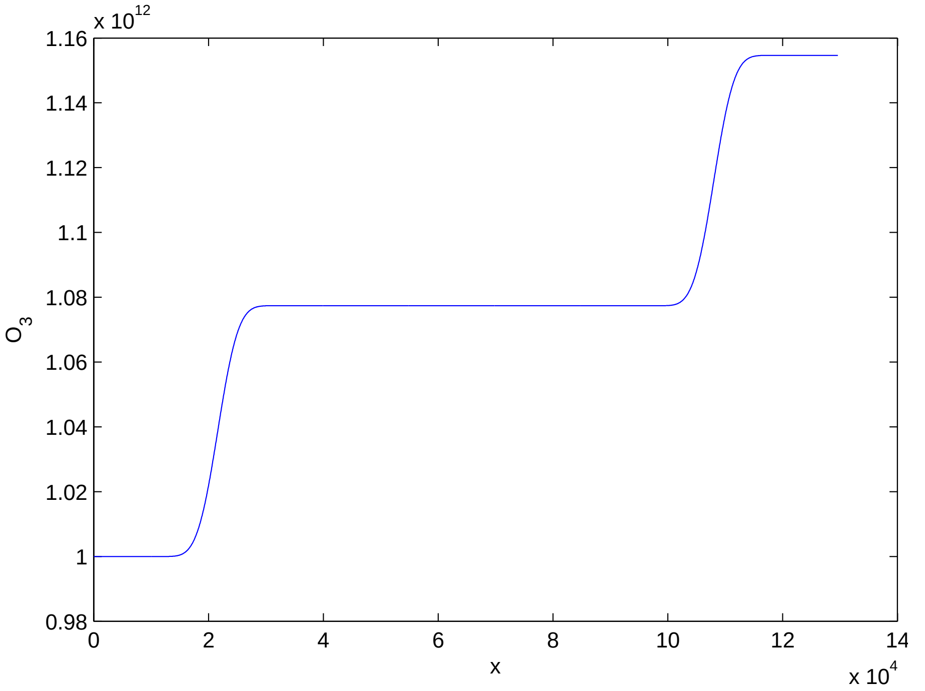

Figure 26: Ozone distribution within the system

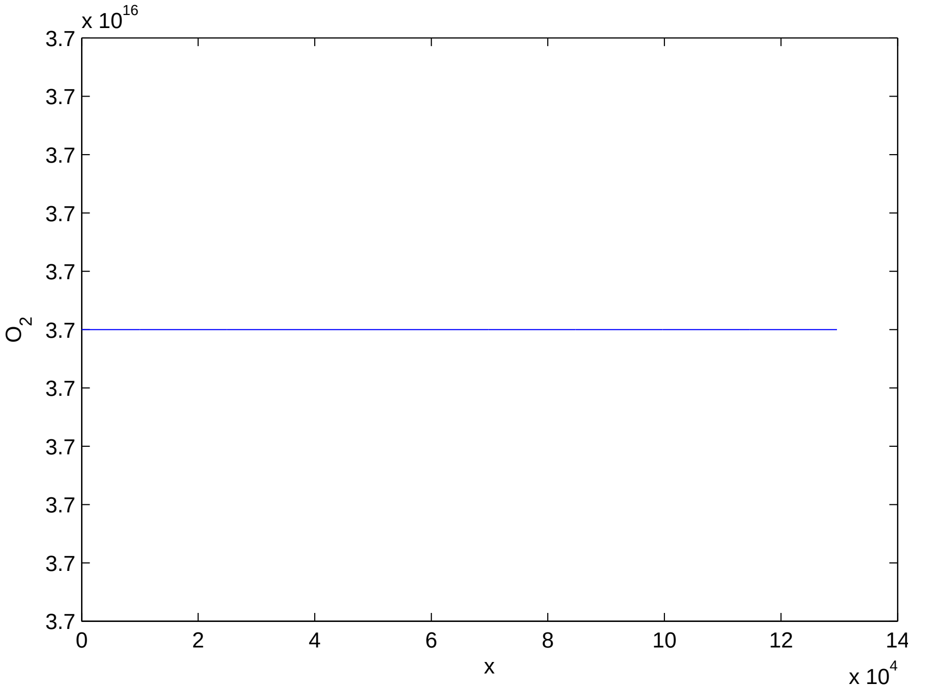

Figure 27: Oxygen gas in the ozone model

The Figure 25 shows that during the daytime there are rapid changes of the concentrations. For instance $[O]$ goes from its initial value to small value for the first seconds, increases to almost 10^8 around noon but then fall off again, while in Figure

26, $[O_3]$ shuts up around noon. During the night both $[O]$ and $[O_3]$ are essentially constant and the process begins again the next morning when the sun rises. Figure 27 shows that $[O_2]$ remain constant throughout, because of its higher order of magnitude than $[O]$ and $[O_2]$. The following figures indicate some solutions of the gases in the ozone system simulated with particle transport method along the computational domain by varying the parameters of the equation 70 and zero income or inflow at the boundary point.

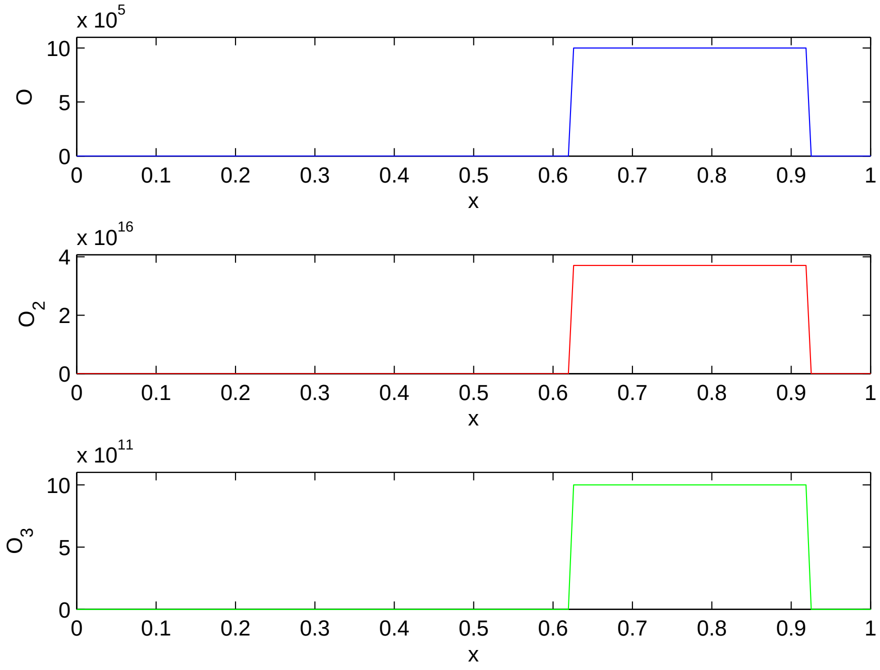

Figure 28: Convection subproblem solution at $t = 3.2$

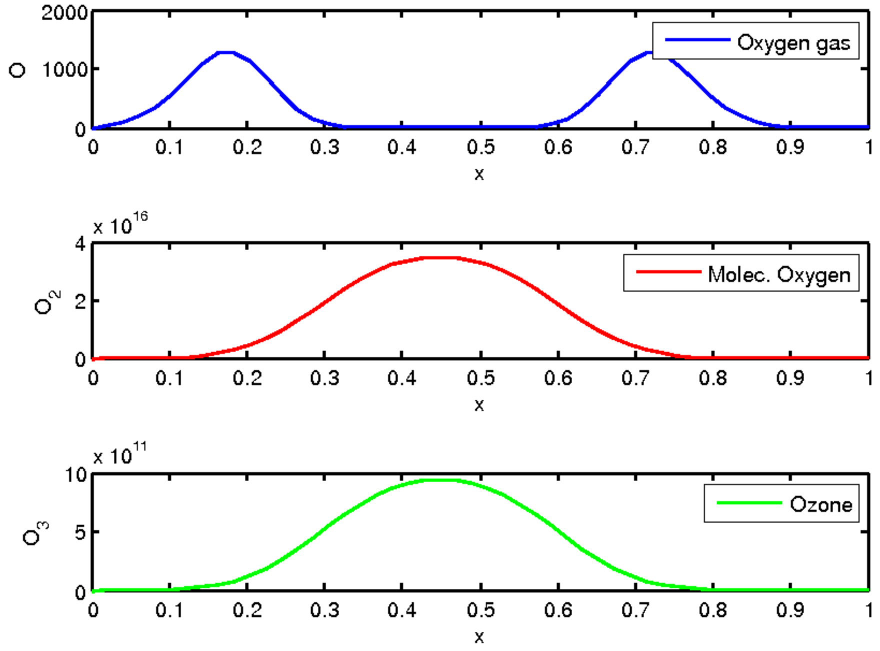

Figure 29: Diffusion-reaction solution at $t = 3.2$

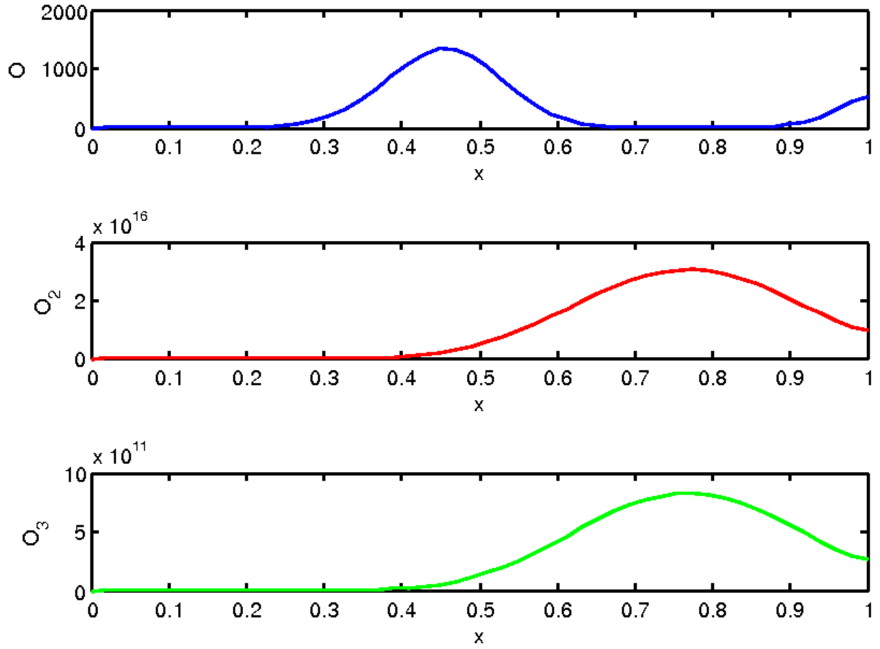

Figure 30: Convection-diffusion-reaction solution at $t = 3.2$

Figure 28, simulated with $D = 0.0, k_1 = 0, k_2 = 0, k_3(t) = 0, k_4(t), u = 0.1$ and $\Delta t = 0.032$, Figure 29 simulated with $D = 0.001, u = 0.0$, $\Delta t = 0.032$ and non zero reaction rates while figure 30 simulated by using $D = 0.001$, $u = 0.1$, $\Delta t = 0.032$ and non zero reactions. Moreover, figures $31 - 33$ involve the flow conditions at the boundary point with the same parameters as the previous problem.

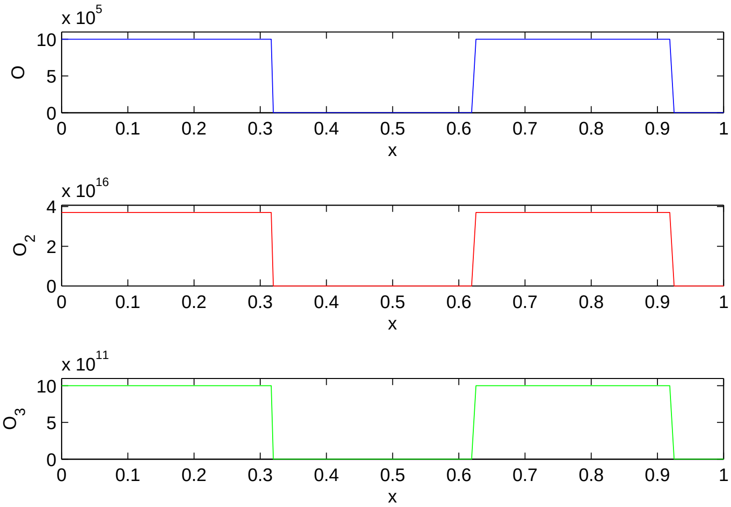

Figure 31: Convection subproblem solution at $t = 3.2$ with inflow

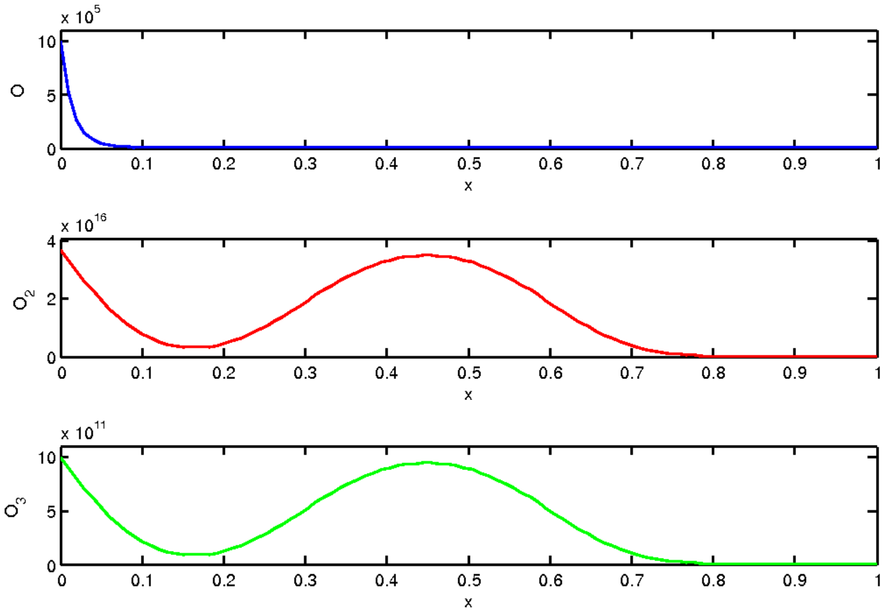

Figure 32: Diffusion-reaction solution at $t = 3.2$ with inflow

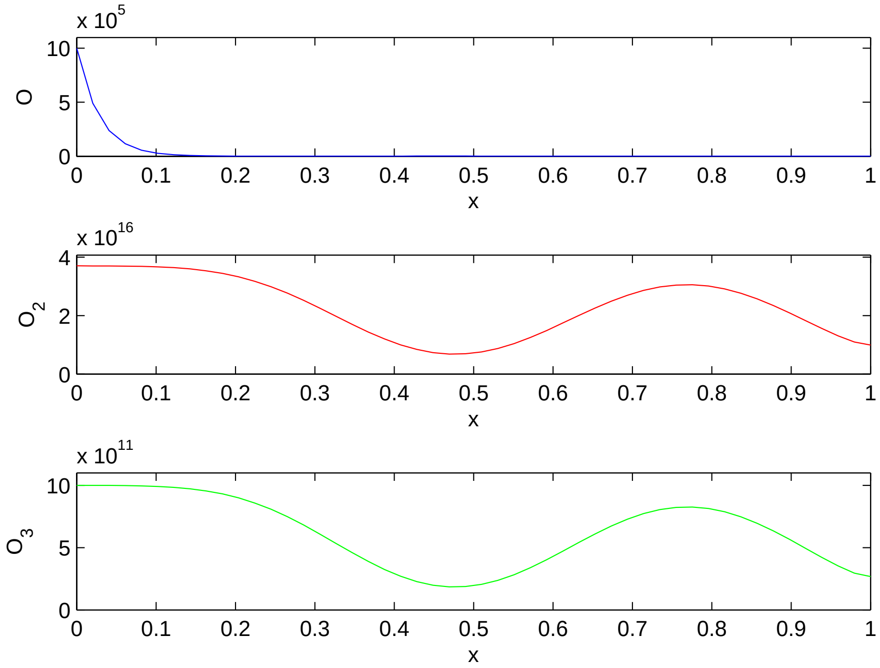

Figure 33: Convection-diffusion-reaction solution at $t = 3.2$ with inflow

As stated in section 4.2, the particle transport method eliminates any artificial oscillations that may occur on the approximated solutions as shown in Figures $28 - 33$. Furthermore, the developed technique (PTM) should be an appropriate technique for the problems that involve moving steep fronts, e.g., pure convective problems due to the fact that, the method controls the resolution of steep fronts and discontinuity to the approximated solution.

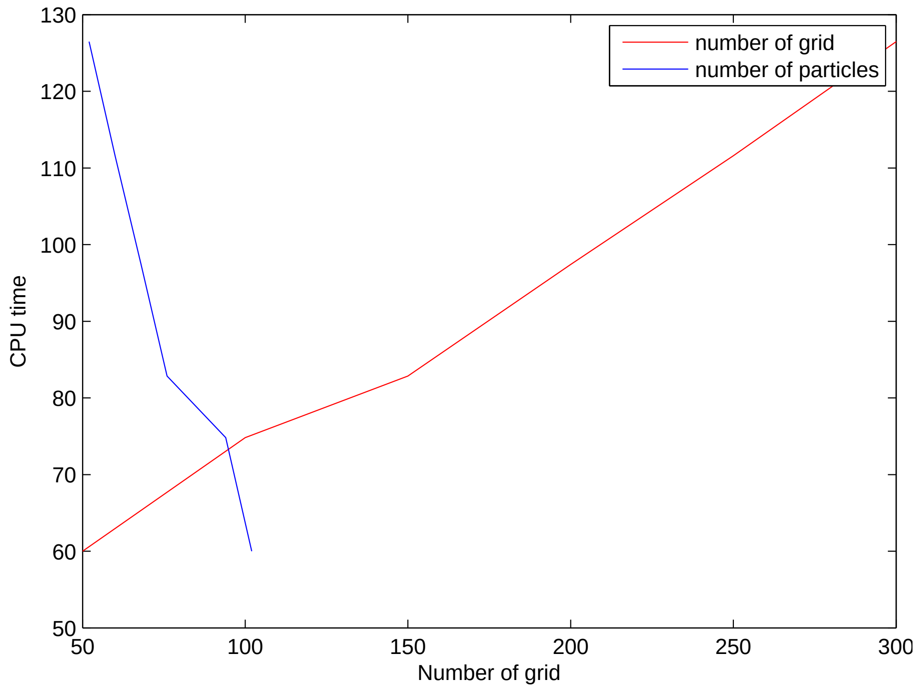

Figure 34: Execution time of particle transport method for the ozone problem

The Figure 34, shows that as the number of grid points along the computational domain increase, the computational time increase too (table 3). This implies that the computational time in second using PTM depends on the number of grid points generated in the domain. Therefore, PTM is an accurate technique in computation of partial differential equations because, it eliminates all difficuities associated with classical methods e.g., Eulerian schemes.

Table 2: Errors at t = 0.04

position of grid	error	position of grid	error
1	0.0001	26	0.0144
2	0.0003	27	0.0154
3	0.0004	28	0.0163
4	0.0003	29	0.0172
5	0.0002	30	0.0179
6	0.0000	31	0.0185
7	0.0003	32	0.0190
8	0.0005	33	0.0193
9	0.0009	34	0.0194
10	0.0012	35	0.0194
11	0.0016	36	0.0191
12	0.0021	37	0.0186
13	0.0027	38	0.0179
14	0.0033	39	0.0169
15	0.0039	40	0.0158
16	0.0047	41	0.0144
17	0.0054	42	0.0129
18	0.0063	43	0.0112
19	0.0072	44	0.0095
20	0.0082	45	0.0078
21	0.0092	46	0.0061
22	0.0102	47	0.0047
23	0.0113	48	0.0036
24	0.0123	49	0.0028
25	0.0134	50	0.0025

Table 3: Computational time (s) for ozone problem with variation of grid number

Number of grid	number of added particles	computational time (CPU time) in seconds
50	102	59.99
100	94	74.82
150	76	82.85
200	68	97.42
250	60	111.60
300	52	126.48

CHAPTER FIVE

CONCLUSION, RECOMMENDATIONS AND THE WAY FORWARD

5.1 Conclusion

In this thesis a general introduction to the models have been described by providing some expositions of analytical and numerical techniques, and the way they do approximate the solutions of the models. This was to give insight of the problem and the general understanding of the models considered.

The literature review gives general ideal and concept of works related to the problem of the study (convection diffusion reaction problem). The idea of characteristics, Lax-Wendroff method, upwind schemes, Lax-Friedrichs schemes, method of lines, meshless methods and sequencing method have been reviewed as well.

The strategy or method of computing CDR problem was analyzed by combining both particle set and fixed-grid points on the same computational area or domain. In this thesis we have considered three kinds of models which are approximated by particle transport method. The first model was considered to have only one component with strong convection and diffusion processes and its solution which is computed by PTM at each time step was compared with the solution by MOL. Second, the non-stiff chemical reaction with three elements was also analyzed using PTM together with MOL. Lastly, the stiff chemical reaction (ozone problem) was solved by including different chemical rates. Meanwhile, the source of artificial oscillation generated by some numerical methods in steep fronts of the moving system has been solved by applications of adaptivity and projection technique. The adaptivity procedure leads to high resolution on the solution due to the addition of moving particles at the initial stage and at the inflow boundary. The transport of the particles along the characteristics is performed by solving the first order Cauchy problem with Runge-kutta method. Then, each particle can be traced with its own accuracy, along the computational domain. Furthermore, we have established the existence of deviation between two solutions which are computed by PTM and MOL in each grid point after every simulation. Therefore, PTM is very efficient numerical technique especially for the problem with steep fronts and discontinuity as the numerical comparisons show; however, in our numerical experiments it is significantly slow when compared with method of lines. As one of the achievement technique in computational of fluid dynamics (CDR), we hope that this thesis will add to the attraction of more students and researchers to study PTM in two, three or more dimensional domain.

5.2 Recommendations

The knowledge about MATLAB software should be insisted if one want to employ particle transport method in the computational process. This will help a learner or a researcher to manage in the process of analyzing the solution of the system at any time interval.

5.3 The way forward

- To apply the particle transport method to the ozone problem with non-constant convective field.

- To apply particle transport method in computational of CDR model with complex domain.

- Use particle transport method to compute a solution of the CDR model with more than four elements in the computational domain.

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